

# **KnowItAll Software Training**

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## Drawing Structures and Reactions

# Drawing Structures and Reactions

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## 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.

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### 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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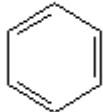



### Background

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



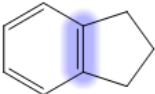



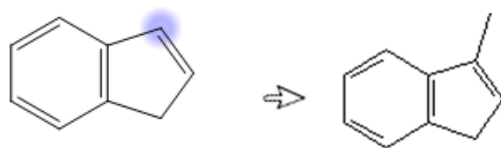
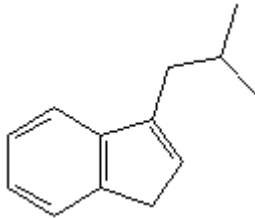
#### *KnowItAll Applications Used*

- ChemWindow®

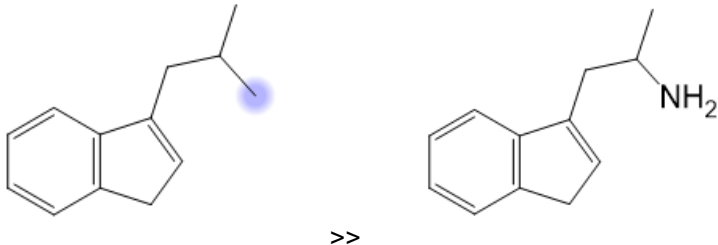
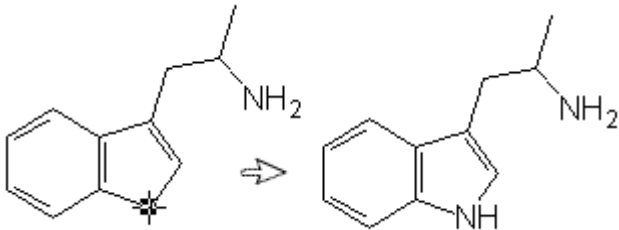
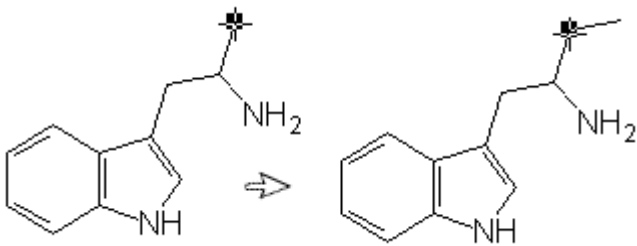
## Begin a new structure drawing

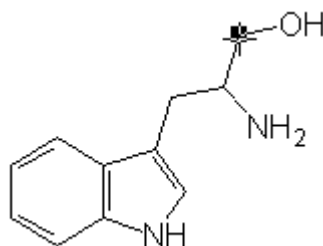
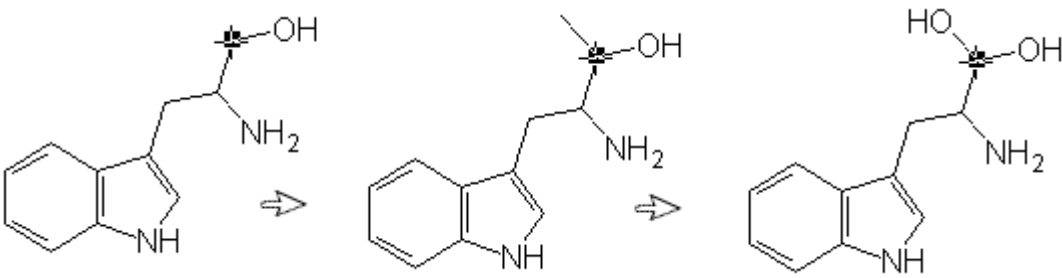
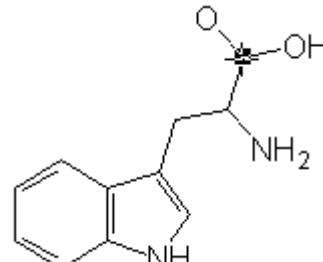
	Action	Result
1	Click the <b>ChemWindow</b> icon in the <b>Basics</b> toolbox.	The <b>ChemWindow</b> application opens to a blank drawing pane.
2	Select the <b>Benzene Ring</b> tool  in the <b>Main</b> section of the <b>Chemistry Toolbar</b> .	
3	Move the cursor into the drawing area, then click to draw 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.  <b>Note:</b> Choose <b>View &gt; Zoom Toolbar</b> to toggle the toolbar display.   The <b>ctrl</b> + <b>scroll</b> function can also be used to zoom in and out quickly.	
5	Use the <b>Selection</b> tool  to select the structure and move it within the workspace.	Graphic handles appear when the structure is selected. 

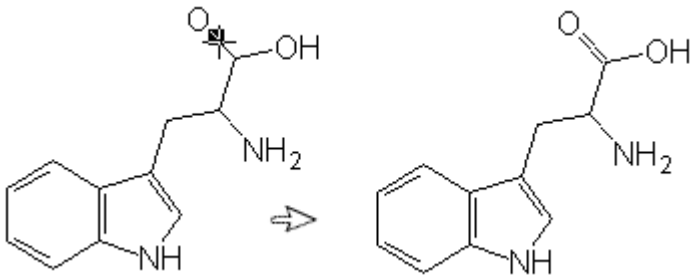
## Add features to the structure

	Action	Result
1	Select the <b>Cyclopentane</b> 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 <b>Bonds</b> group in the <b>Drawing Toolbar</b> and select the <b>Inside Double Bond</b> tool  . Then use it to add a double bond to the structure.	
4	Select the <b>Single Bond</b> tool  . Then move the cursor over the atom's hit box as shown. Click to create a single bond.	 <b>Note:</b> 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.	

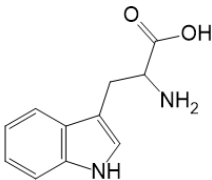
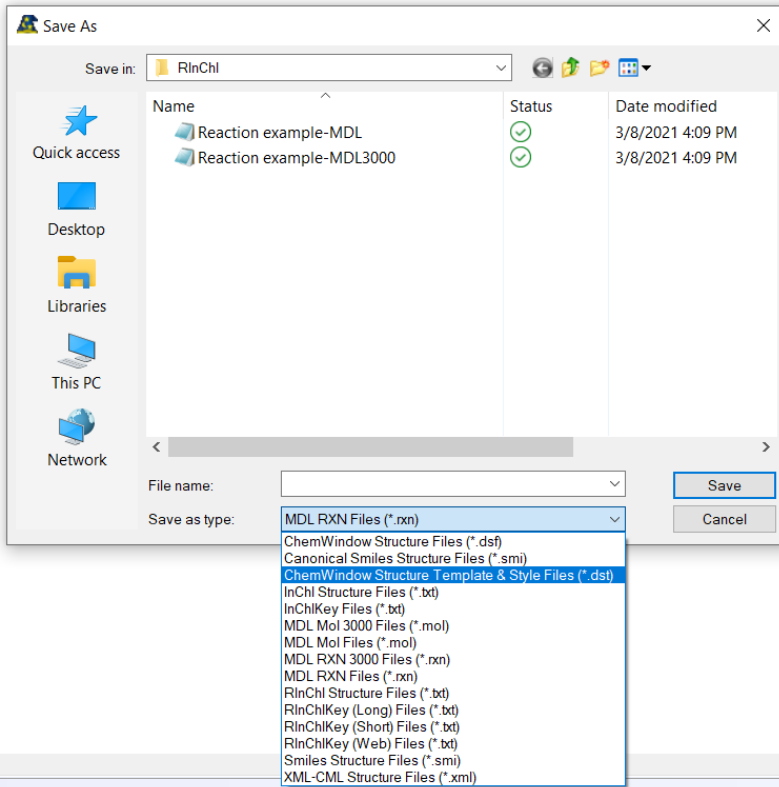
**Use hot keys to add nitrogen and oxygen atoms**

	Action	Result
1	Move the cursor over the terminal carbon. Then press <b>n</b> (not <b>nh</b> ) on your keyboard.	<p><b>NH<sub>2</sub></b> appears at the end of the bond.</p>  <p><b>Note:</b> 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 <b>NH</b> .	
3	With the single bond tool still selected, place your cursor over the terminal carbon atom and click to add another single bond.	

	Action	Result
4	Without moving the cursor, press <b>o</b> on your keyboard.	 The diagram shows the chemical structure of tryptamine (3-(2-aminoethyl)indole). A cursor is positioned on the alpha carbon of the ethyl side chain. An OH group is being added to this carbon, indicated by a bond extending from the cursor to the OH group.
5	Click to sprout another single bond.  Then press <b>o</b> on the keyboard to add a hydroxyl group.	 The diagram illustrates the step-by-step addition of a second hydroxyl group. It shows three stages: 1) The initial tryptamine structure with a cursor on the alpha carbon. 2) A single bond is sprouted from the alpha carbon. 3) A hydroxyl group (HO) is added to the sprouted bond, resulting in a 1,1-dihydroxyethyl side chain.
6	Press <b>o</b> again to remove the hydrogen.  <b>Note:</b> When using a hot key, you can change the number of hydrogens attached to the atom by pressing the hot key repeatedly.	 The diagram shows the final structure where the alpha carbon is part of a carboxylic acid group. The hydrogen atom previously attached to the alpha carbon has been removed, and a double bond to an oxygen atom (O) has been formed, resulting in a tryptophan derivative.


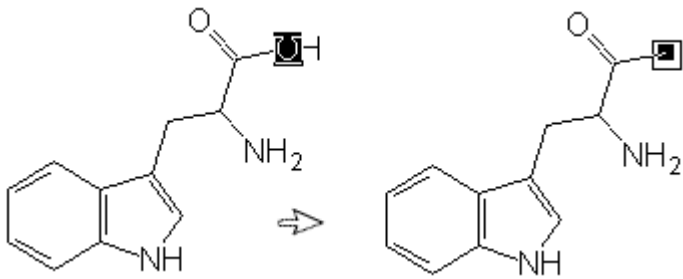
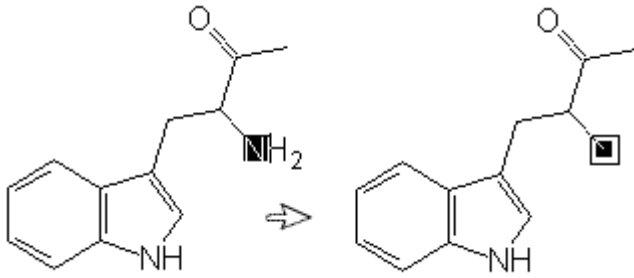

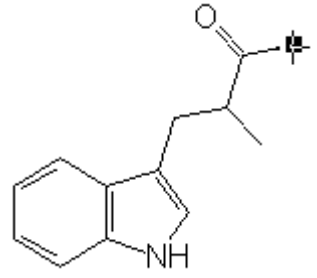
	Action	Result
7	Move the cursor to the hit box on the bond. Then click to create a double bond.	

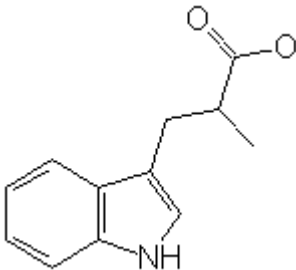


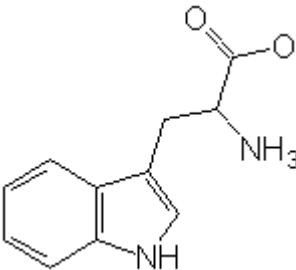

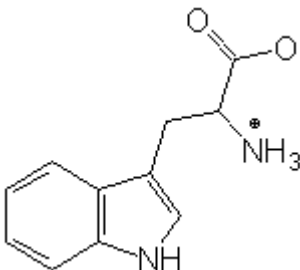
## Save the structure


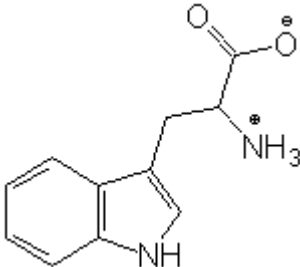
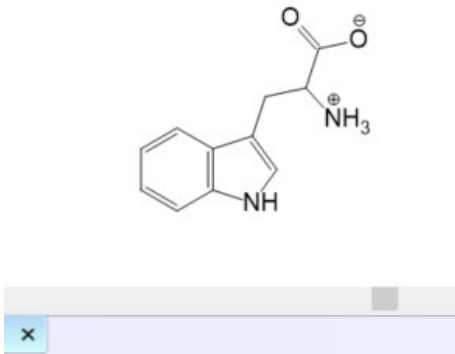
	Action	Result
1	<p>Choose <b>File &gt; Save</b>.</p> <p><b>Note:</b> You can also click the <b>Save</b> button on the toolbar or press Ctrl+S.</p>	<p>The <b>Save As</b> dialog box opens. The default file type (<b>ChemWindow</b> structure file, *.dsf) is already selected, and will be used for this structure.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



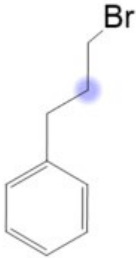
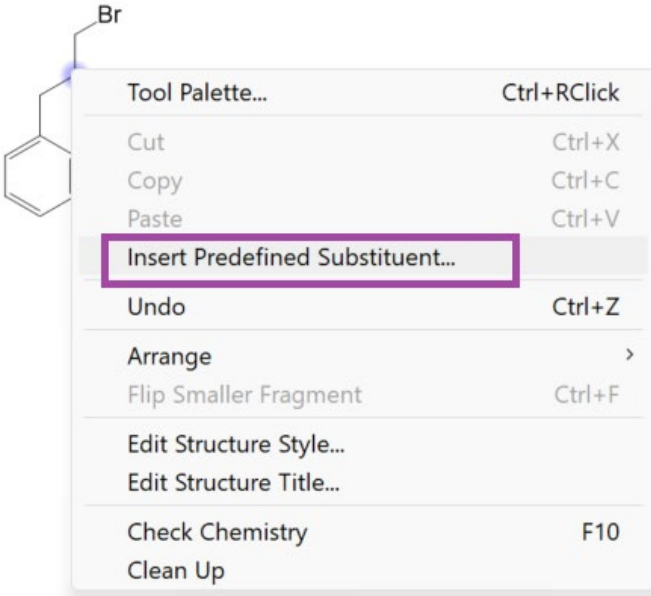
**Edit the structure and use atom labels and atom tags**

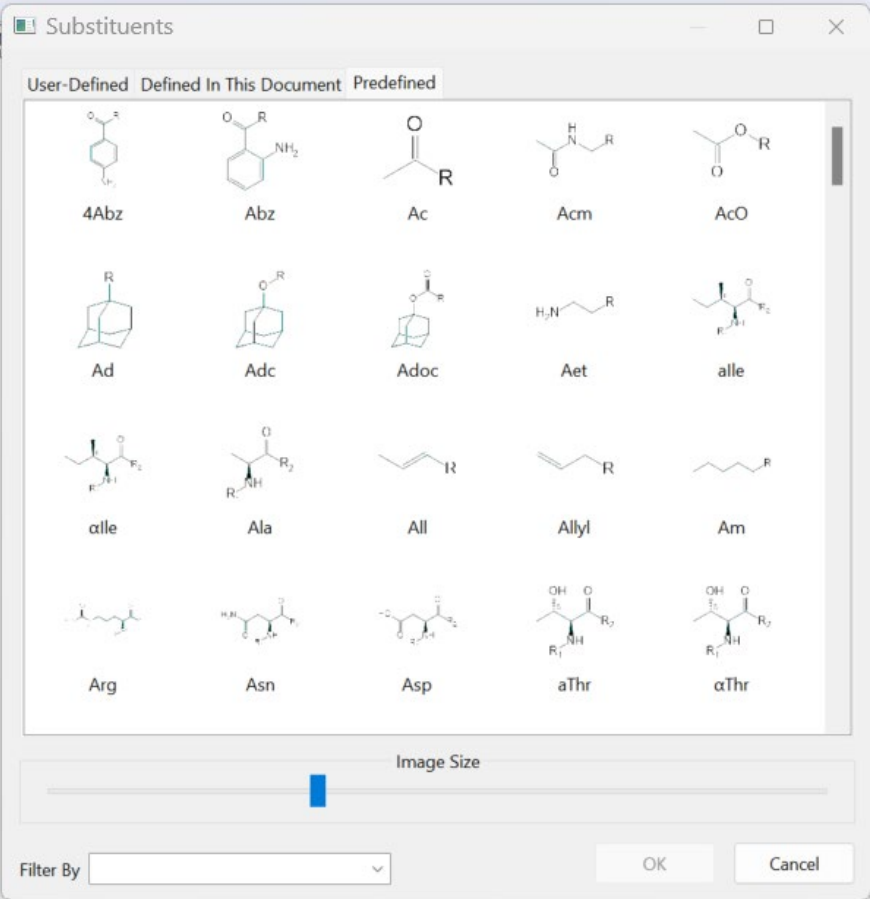
	Action	Result
1	Select the <b>Eraser</b> tool  , then click to remove the hydroxyl.	
2	Click to remove amino groups.	
3	Open the <b>Main</b> group on the <b>Drawing Toolbar</b> and select the <b>Atom Label</b> tool  . Then click where the hydroxyl group was located.	

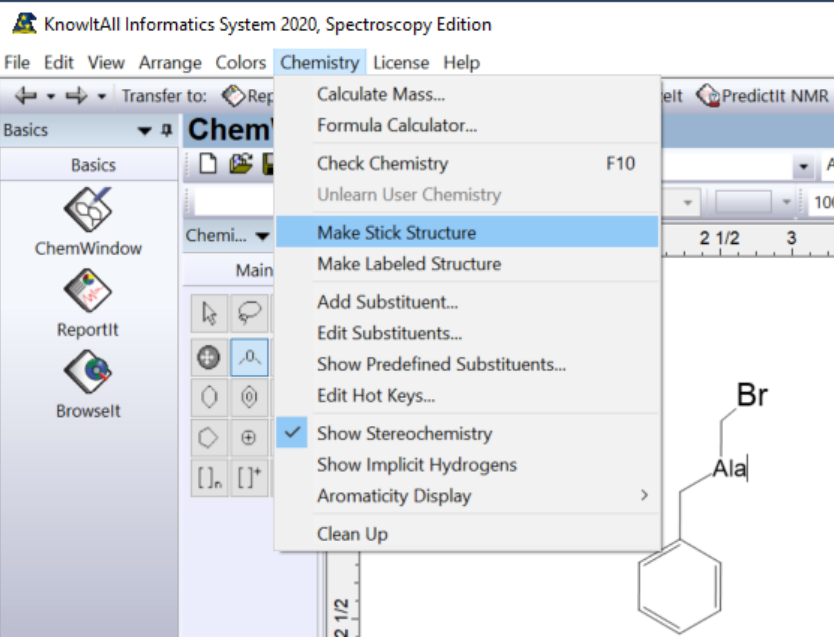
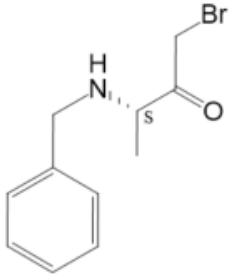
	Action	Result
4	Type uppercase <b>O</b> .  <b>Note:</b> Atom labels are case-sensitive.	
5	Move to the other atom and type uppercase <b>NH3</b> .  <b>Note:</b> Numbers are automatically displayed as subscripts if the <b>Text</b>  is selected.  <b>Style</b> toolbar's <b>Formula</b> tool  is selected.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

	Action	Result
7	Repeat with the <b>Negative Charge Atom Tag</b> tool  to add a negative charge to the oxygen atom.	
8	Choose <b>File &gt; Save As</b> to save the structure with file name <b>tryptophan2.dsf</b> .	
9	Click the "x" at the bottom tab to close this drawing  Click <b>No</b> at saving file prompt  This would start a new blank ChemWindow screen.	

**Use pre-defined substituents**

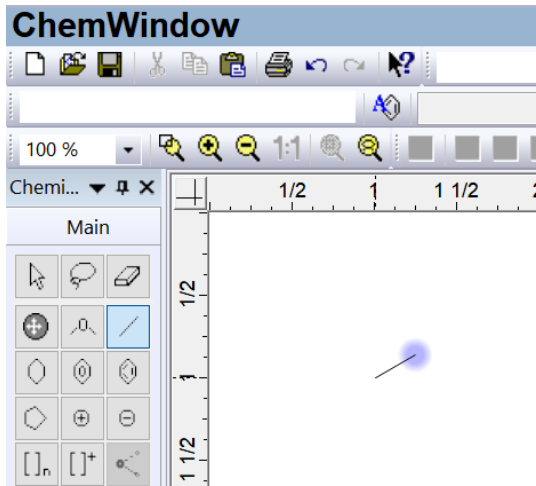
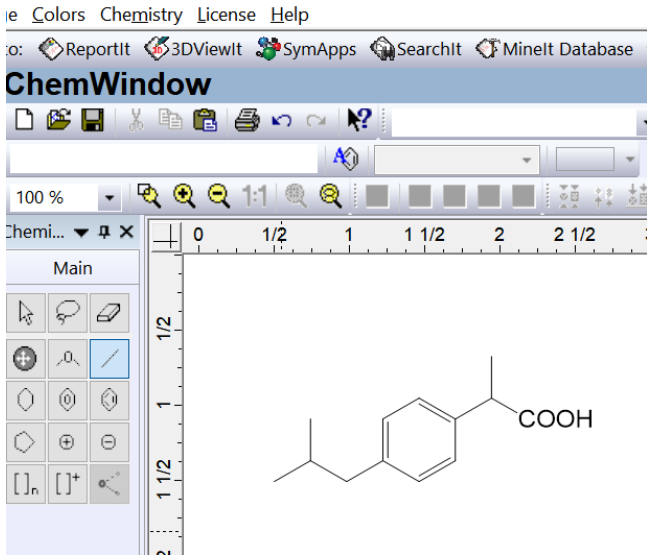
	Action	Result
1	<ul style="list-style-type: none"><li>• Draw the structure shown</li><li>• Mouse over the atom (it is highlighted)</li></ul>	
2	<ul style="list-style-type: none"><li>• Right-mouse-click to bring up menus</li><li>• Choose <b>Insert Pre-defined Substituent</b></li></ul>	

	Action	Result
3	<ul style="list-style-type: none"><li>Pick <b>Ala</b></li><li><b>OK</b></li></ul>	<p>A table shows all predefined substituents. One can sort the contents using <b>Filter By</b>:</p>  <p>Note: there is another way to achieve this – after one highlights the atom in step 2, one can type in <b>Ala</b>, this does require one to know what 3 letters to use.</p>

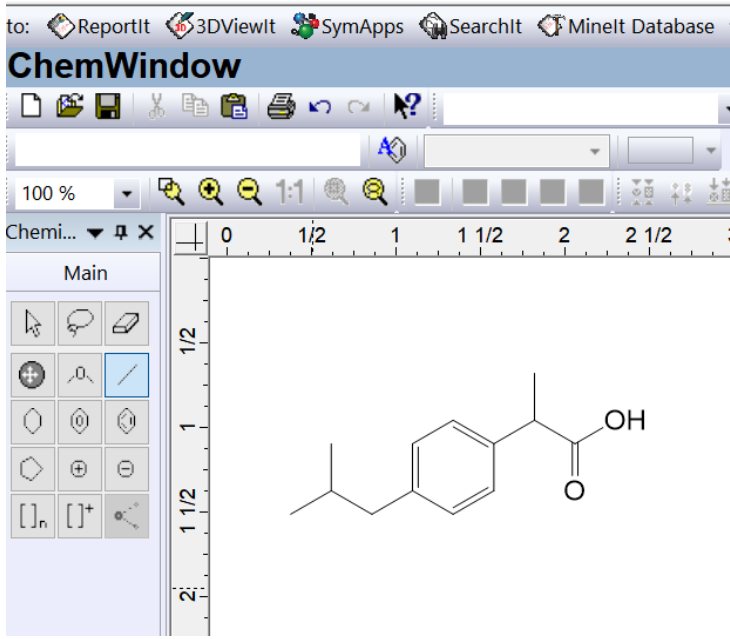
	Action	Result
4	Click <b>Chemistry &gt; Make Stick Structure</b> .	
5		 <p data-bbox="716 1271 1108 1299">The above is the expanded structure.</p>

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

## Use Hotkeys

	Action	Result
1	<p>In the Main toolbox, select the <b>Standard bond</b> tool.</p> <p>Click the structure pane to insert the single bond. The end of the bond will be highlighted automatically.</p>	
2	<p>Type the following characters on your keyboard: 9, 1, 3, 9, shift + O (Capital letter O).</p> <p>(Note that hot keys involving capital letters use shift + letter, not caps lock + letter.)</p>	

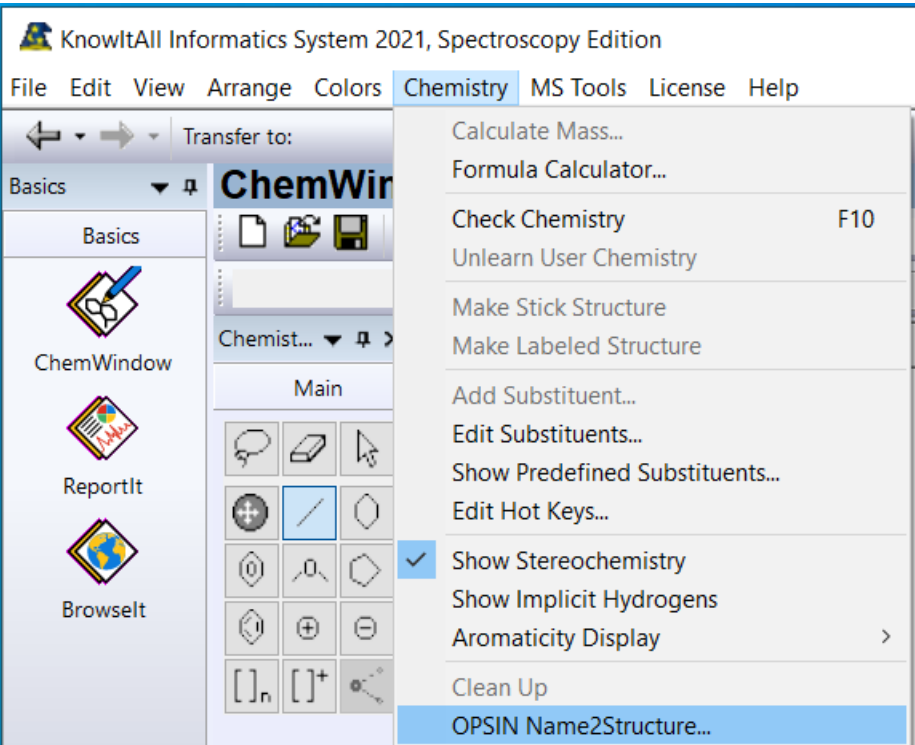


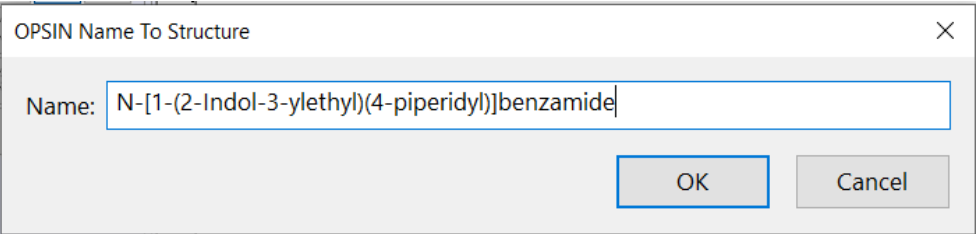
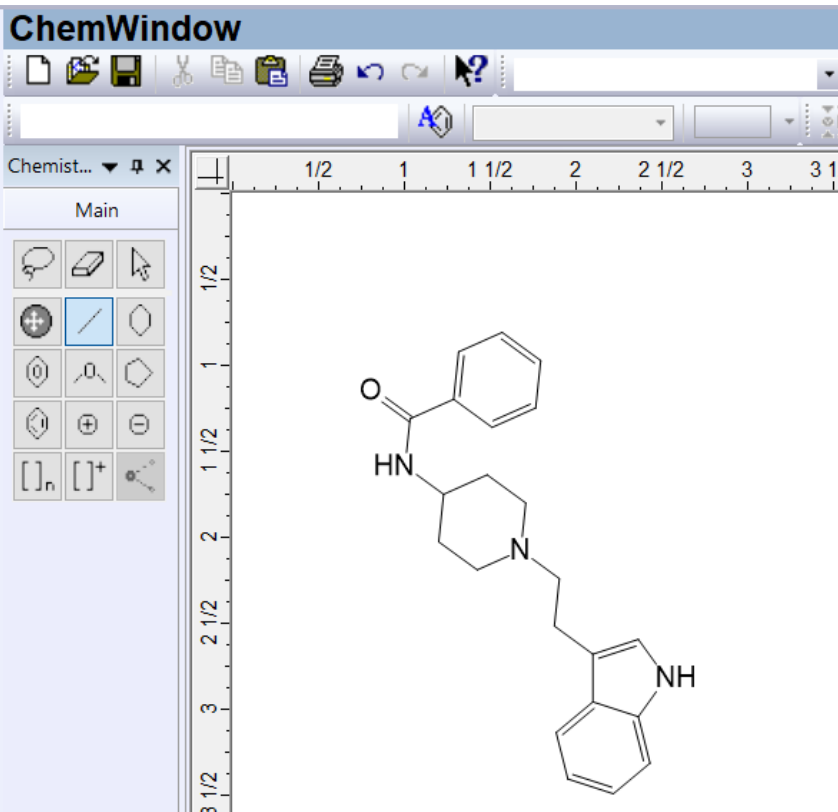
	Action	Result
3	Click <b>Chemistry &gt; Make Stick Structure</b> .	 <p>The above is the expanded structure.</p>
4	Click the "x" at the bottom tab to close this drawing.  Click <b>No</b> at saving file prompt.  This would start a new blank ChemWindow screen.	

**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 <b>Chemistry &gt; OPSIN Name2Structure</b> .	

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

	Action	Result
4	Click the "x" at the bottom tab to close this drawing  Click <b>No</b> at saving file prompt  This would start a new blank ChemWindow screen.	

### 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

### 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**

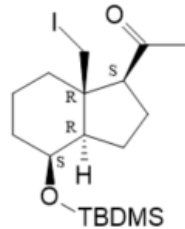
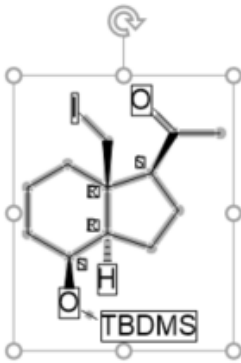
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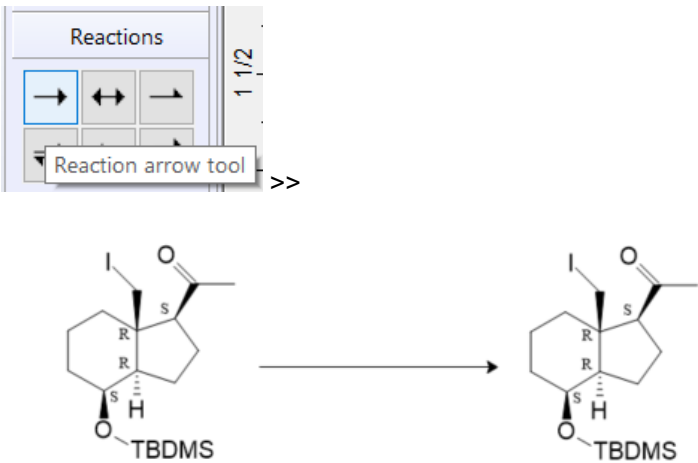
- Reactant.dsf

#### **KnowItAll Applications Used**

- ChemWindow®

## Draw Chemical Reactions

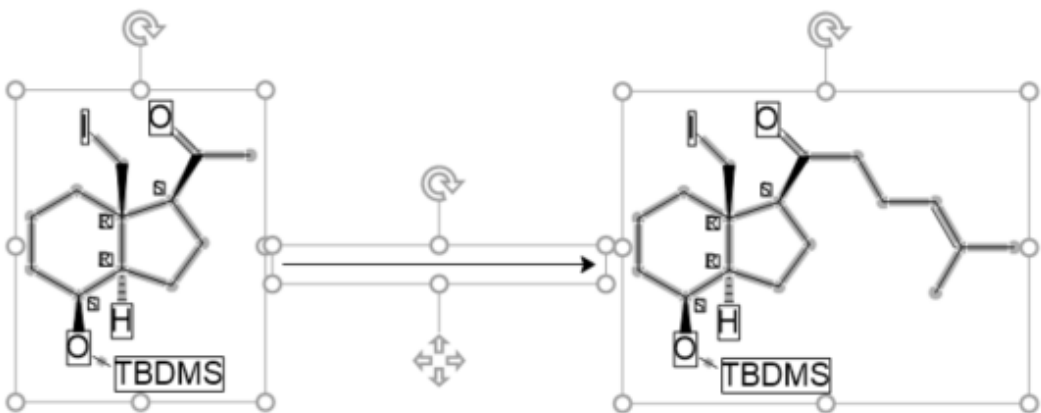
	Action	Result
1	Click the <b>ChemWindow</b> icon in the <b>Basics</b> toolbox.	The ChemWindow application opens to a blank drawing.
2	Navigate to <b>File &gt; Open</b> , then navigate to <b>C:\Users\Public\Documents\Wiley\KnowItAll\Samples\Reactions</b> .  Select <b>Reactant.dsf</b> .  Click <b>Open</b> .	The file opens in the workspace.   <p>The chemical structure is a bicyclic compound consisting of a cyclohexane ring fused to a cyclopentane ring. The cyclohexane ring has an iodine atom (I) at the top position and a TBDMS-protected alcohol group (O-TBDMS) at the bottom position. The cyclopentane ring has a ketone group (C=O) at the top position. Stereochemistry is indicated with 'R' and 'S' labels and wedged/dashed bonds.</p>
3	Select the structure.	 <p>The chemical structure is shown within a selection box, indicating it has been selected for editing. A rotation handle is visible at the top of the box.</p>

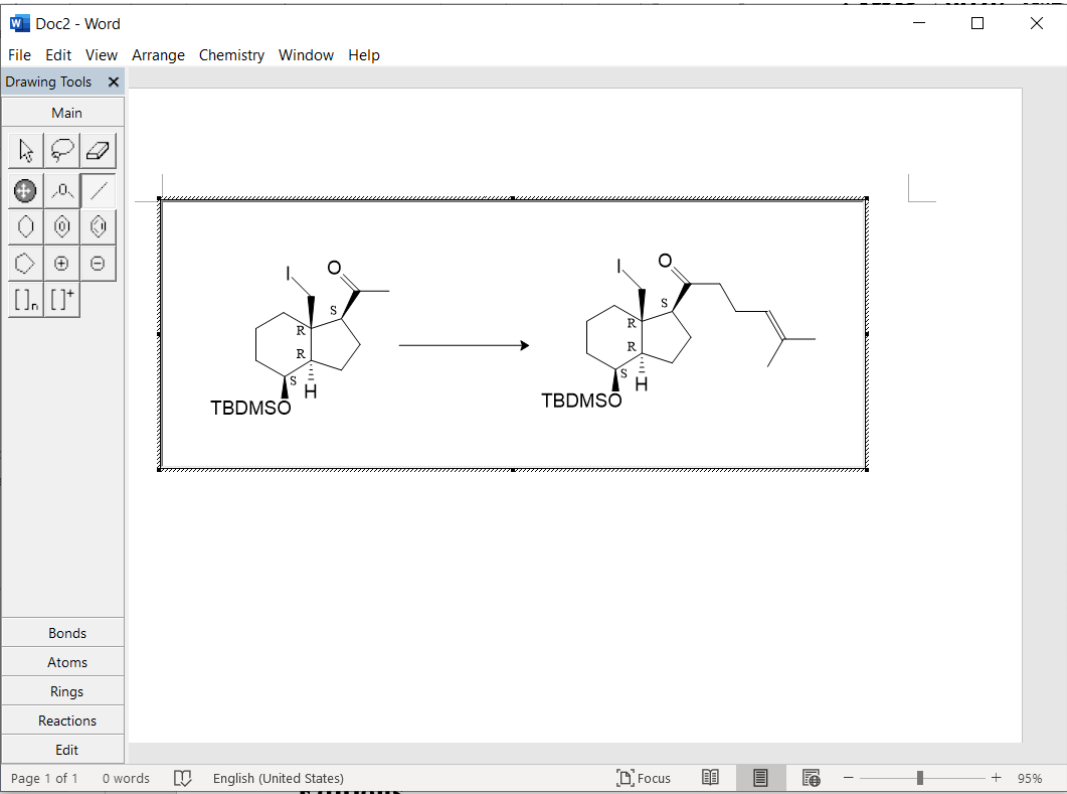
	Action	Result
4	Navigate to <b>Edit &gt; Copy</b> , then <b>Edit &gt; Paste</b> .	
5	In the <b>Reactions</b> toolbox, select <b>Reaction arrow</b> tool and draw between the two structures.	

	Action	Result
6	Modify the structure on right to be the product.	<p>The diagram shows a chemical reaction. On the left is the starting material, a bicyclic ketone. It consists of two fused six-membered rings. The left ring has a ketone group (=O) and a tert-butyldimethylsilyl (TBDMS) ether group (-OTBDMS) on the same carbon. The right ring has a ketone group (=O) and an iodine atom (I) on the same carbon. An arrow points to the right, leading to the product. The product is a bicyclic enone, where the ketone group on the right ring has been converted to an enone group (=C-C=C-CH<sub>3</sub>), and the iodine atom remains on the same carbon. The stereochemistry of the other groups remains unchanged.</p>

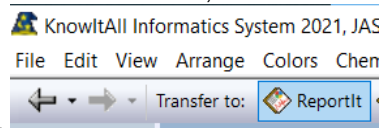


**OLE connection with MS Office tools**

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

	Action	Result
3	In the MS Word document, double-click on the KnowItAll object saved.	<p>You can perform ChemWindow actions from here.</p>  <p><b>TIP:</b> You can work with other MS office tools in the same way.</p>

**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.

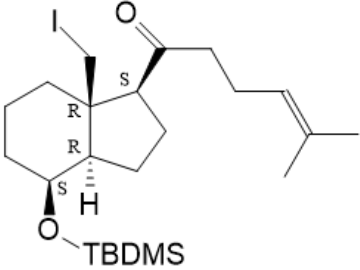
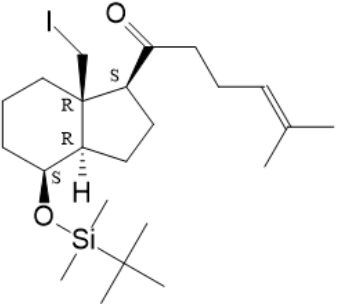
#### *Training Files Used in This Lesson*

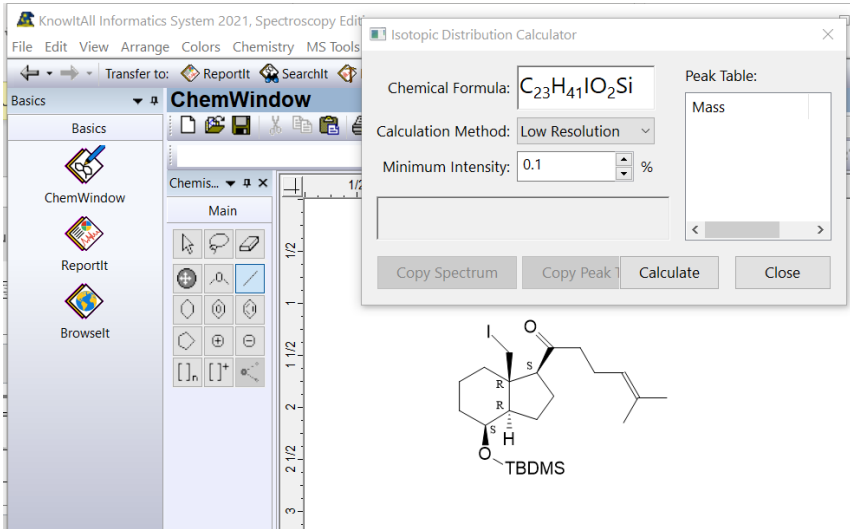
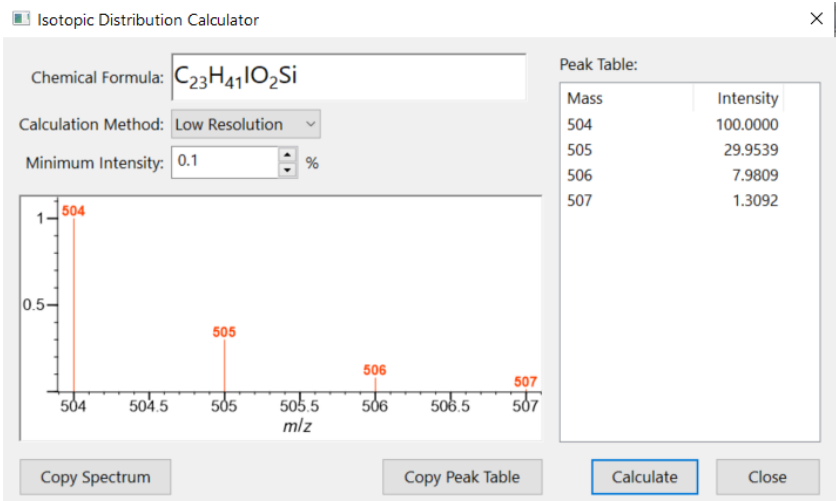
- Structure 2.dsf

#### *KnowItAll Applications Used*

- ChemWindow®

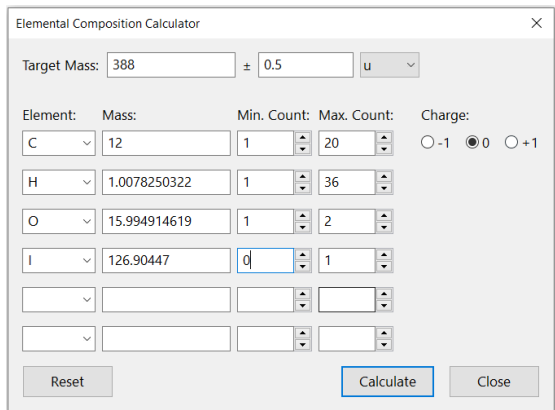
## Isotopic Distribution

	Action	Result
1	<p>Navigate to <b>File &gt; Open</b>, then navigate to <b>C:\Users\Public\Documents\Wiley\KnowItAll\Samples\Reactions</b> folder.</p> <p>Select <b>Product.dsf</b>.</p> <p>Click <b>Open</b>.</p>	 <p>The chemical structure shows a bicyclic system consisting of a cyclohexane ring fused to a cyclopentane ring. The cyclohexane ring has an iodine atom (I) at the top position and a tert-butyldimethylsilyl (TBDMS) ether group at the bottom position. The cyclopentane ring has a ketone group (C=O) at the top position and a hydrogen atom (H) at the bottom position. The stereochemistry is indicated with R and S labels at the chiral centers.</p> <p>You can calculate Isotopic Distributions for a database record structure.</p>
2	<p>Navigate to <b>Chemistry &gt; Make Stick Structure</b>.</p>	 <p>The chemical structure is identical to the one in step 1, but the TBDMS group is represented using a stick model for the tert-butyl and dimethyl groups, while the silicon atom (Si) and oxygen atom (O) are shown as circles.</p>

	Action	Result										
3	<p>Navigate to <b>MS Tools &gt; Calculate Isotopic Distribution</b>.</p> <p>In the pop-up window, click <b>Calculate</b>.</p>	 <p>Chemical Formula: <math>C_{23}H_{41}IO_2Si</math></p> <p>Calculation Method: Low Resolution</p> <p>Minimum Intensity: 0.1 %</p> <p>Peak Table:</p> <table><tr><th>Mass</th><th>Intensity</th></tr></table> <p>Buttons: Copy Spectrum, Copy Peak Table, Calculate, Close</p>	Mass	Intensity								
Mass	Intensity											
4		 <p>Chemical Formula: <math>C_{23}H_{41}IO_2Si</math></p> <p>Calculation Method: Low Resolution</p> <p>Minimum Intensity: 0.1 %</p> <p>Peak Table:</p> <table><tr><th>Mass</th><th>Intensity</th></tr><tr><td>504</td><td>100.0000</td></tr><tr><td>505</td><td>29.9539</td></tr><tr><td>506</td><td>7.9809</td></tr><tr><td>507</td><td>1.3092</td></tr></table> <p>Buttons: Copy Spectrum, Copy Peak Table, Calculate, Close</p>	Mass	Intensity	504	100.0000	505	29.9539	506	7.9809	507	1.3092
Mass	Intensity											
504	100.0000											
505	29.9539											
506	7.9809											
507	1.3092											
5	Close this dialog											

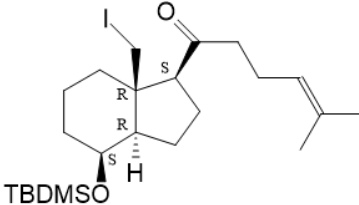
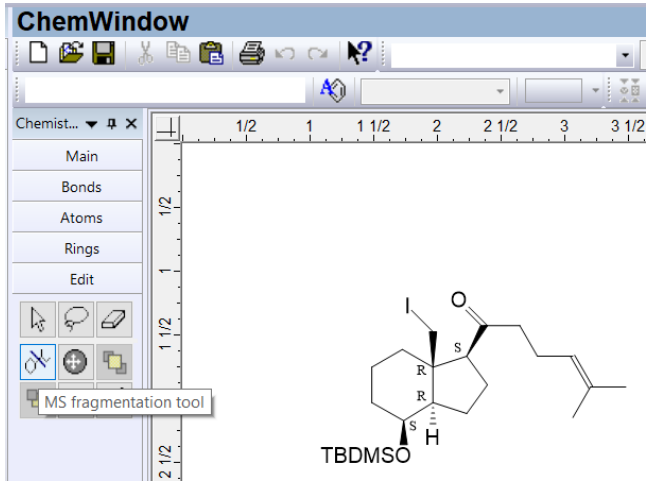
## Isotopic Elemental Composition

This tool is not associated with a database record structure.

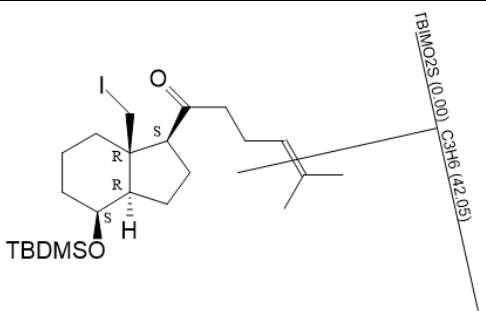
	Action	Results
1	Navigate to <b>MS Tools &gt; Calculate Elemental Composition</b> .	<p>This dialog shows up.</p> 

	Action	Results																																																	
2	Fill in elements and occurrences and click <b>Calculate</b> .	<div>Combinations of elements are displayed.</div> <div><div>Elemental Composition Results</div><div><div>Target Mass: 388 ± 0.5 u</div><div>Charge: 0Result Count: 6</div><table><tr><th>C</th><th>H</th><th>O</th><th>I</th><th>m</th><th>Δm [u]</th><th>Δm [ppm]</th></tr><tr><td>18</td><td>13</td><td>2</td><td>1</td><td>387.9960</td><td>-0.0040</td><td>-10.2457</td></tr><tr><td>19</td><td>17</td><td>1</td><td>1</td><td>388.0324</td><td>0.0324</td><td>83.5314</td></tr><tr><td>20</td><td>5</td><td>1</td><td>1</td><td>387.9385</td><td>-0.0615</td><td>-158.4799</td></tr><tr><td>17</td><td>25</td><td>2</td><td>1</td><td>388.0899</td><td>0.0899</td><td>231.7656</td></tr><tr><td>19</td><td>1</td><td>2</td><td>1</td><td>387.9021</td><td>-0.0979</td><td>-252.2570</td></tr><tr><td>18</td><td>29</td><td>1</td><td>1</td><td>388.1263</td><td>0.1263</td><td>325.5427</td></tr></table></div><div><div>Copy To Clipboard</div><div>Close</div></div></div>	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
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18	29	1	1	388.1263	0.1263	325.5427																																													

## MS Fragmentation

	Action	Results
1	<p>Navigate to <b>File &gt; Open</b>. Then navigate to <b>C:\Users\Public\Documents\Wiley\KnowItAll\Samples\Reactions</b> folder.</p> <p>Select <b>Product.dsf</b>.</p> <p>Click <b>Open</b>.</p>	 <p>You can calculate Isotopic Distributions for a database record structure.</p>
2	<p>In the <b>Edit</b> toolbox, select the <b>MS fragmentation tool</b>.</p>	 <p>The screenshot shows the ChemWindow application window. The title bar reads 'ChemWindow'. Below the title bar is a menu bar with 'Chemist...' and a dropdown arrow. Below the menu bar is a toolbar with various icons. Below the toolbar is a vertical toolbar with buttons for 'Main', 'Bonds', 'Atoms', 'Rings', and 'Edit'. Below the vertical toolbar is a horizontal toolbar with icons for 'MS fragmentation tool', 'MS fragmentation tool', and 'MS fragmentation tool'. The 'MS fragmentation tool' is highlighted. The main window displays the chemical structure of the bicyclic compound.</p>



	Action	Results
3		 <p>You can clip the structure into two fragments.</p>
4	Click <b>Close (X)</b>	