ACD/ChemSketch Technical Note: Advanced Features and Functions

ACD/ChemSketch
Version 2015

Sherry Myles and Arvin Moser
Advanced Chemistry Development, Inc.
Toronto, ON, Canada
www.acdlabs.com

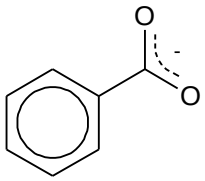
ACD/ChemSketch is a powerful structure drawing and naming software program. This Technical Note highlights several advanced drawing tools that are available in ACD/ChemSketch. A free 30 day trial download of ACD/ChemSketch is available from our web site: www.acdlabs.com/chemsketch/

Advanced Drawing Features

Once you have established how to draw basic structures and use the general features (outlined in our Quick Start Guide www.acdlabs.com/quickstart_chemsketch/) you are ready to explore some of the more advanced features.

Delocalized Bonds

ACD/ChemSketch is capable of correctly representing structures containing delocalized bonds. This section presents the general procedure necessary to draw delocalized bonds using the example on the right.



1. Go to **Structure** mode 

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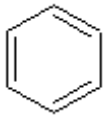
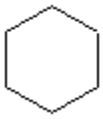
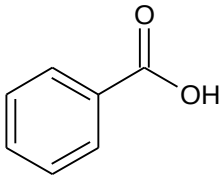
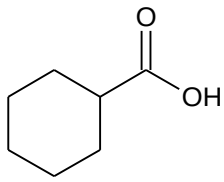
2. From the **Templates** menu, choose **Table of Radicals**, then from the **Table of Radicals** window, select either benzene  or cyclohexane  and paste it in the Structure window.
3. From the **Table of Radicals**, choose 

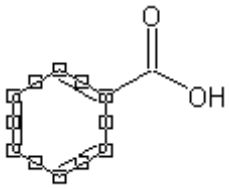
to attach a carboxyl group to the ring. You shall see either of the following structures:



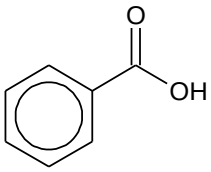
OR



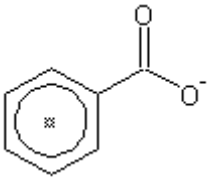
4. Select the benzene or cyclohexane ring by choosing **Select/Move**  and dragging over the substructure.



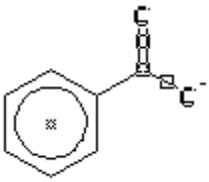
5. Click the **Solid Delocalization Curve** and the structure will look like the below.



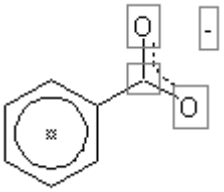
6. Use the **Decrement Charge** button to place a negative charge on the OH group.



7. Select the COO^- group.



8. Click the white triangle on the **Solid Delocalization Curve** button and select the **Dotted Delocalization Curve** option  to get the following structure:



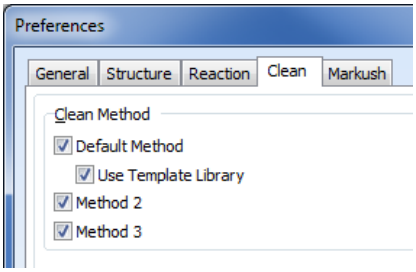
9. The negative sign on the COO^- group can be moved around to the desired area.

> **Note** To show a delocalized bond quickly, draw a benzene ring and then, from the **Tools** menu, choose **Show Aromaticity**.

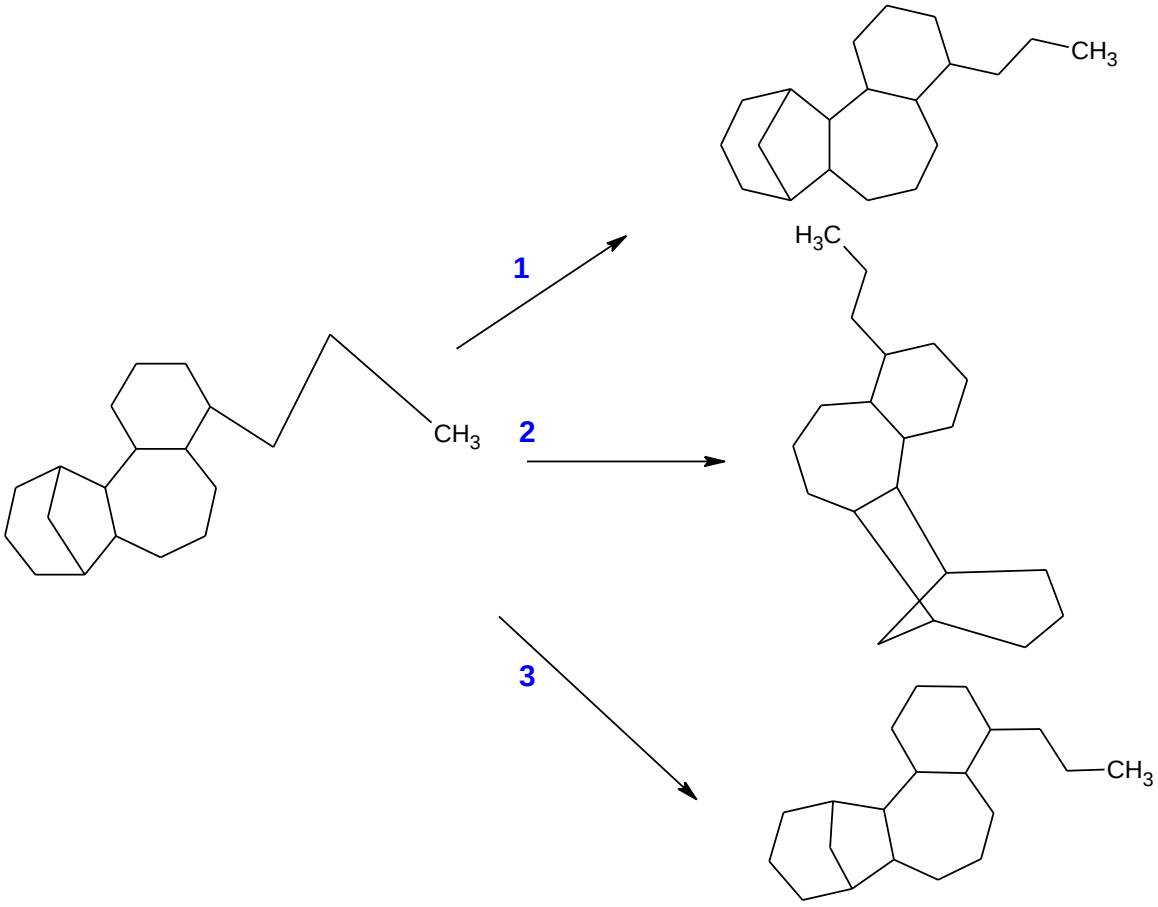
Cleaning Structures

ACD/ChemSketch incorporates three (3) algorithms to quickly standardize bonds and angles and resize structures; which each have their own benefits.

1. You can set your Clean Structure preferences in **Structure** mode. From the **Options** menu, choose **Preferences**. By default all 3 algorithms are enabled.



2. Select your desired structure (if there are multiple structures on a page and you do not select just one, all will be cleaned). Click **Clean Structure** multiple times to cycle through the algorithms: Default, Method 2, and Method 3.



While there is no single, ideal algorithm for cleaning structures, the third method is best suited for most simple and complex molecules. There can be times that the other two algorithms may offer advantages, so we continue to provide all three.

Creating Custom Radical Labels

Use ACD/ChemSketch to add radical labels, with a custom labeling style, to your drawing.

1. From ACD/ChemSketch, draw the desired structure in **Structure** mode 

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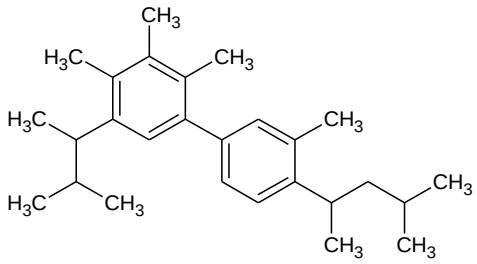
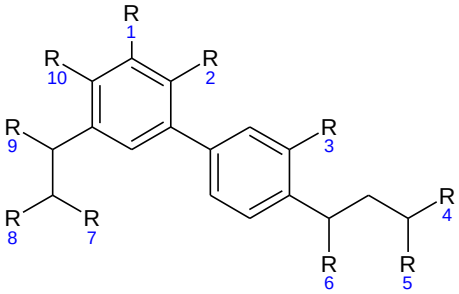


2. Choose the radical drawing tool 

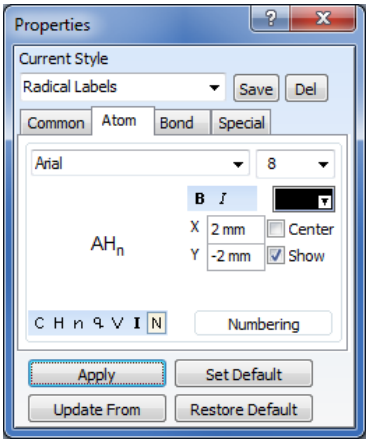
and select the groups that you would like changed to a radical group.
3. After all radicals have been created, choose the manual renumbering tool 

. The Manual Renumbering dialog window will appear. Customize the numbering format to your preference and then choose **OK**. Then click on the "R" labels in order to number them.

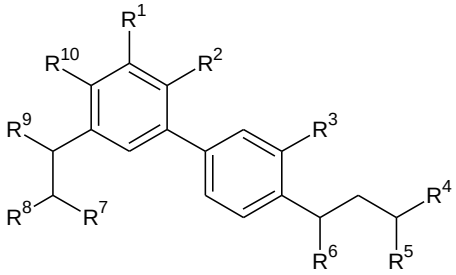


4. Select all the radical labels by holding down **Shift** on the keyboard while left-clicking on the radical labels. Then from the **Tools** menu, choose **Structure Properties**.
5. In the **Properties** dialog box that appears; on the **Atom** tab, choose the **Numbering** button 

to modify the numbering format. Enter a name for this label in the **Current** Style box (i.e., Radical Labels). Set the values as shown below, and be sure to select the **Show** check box.



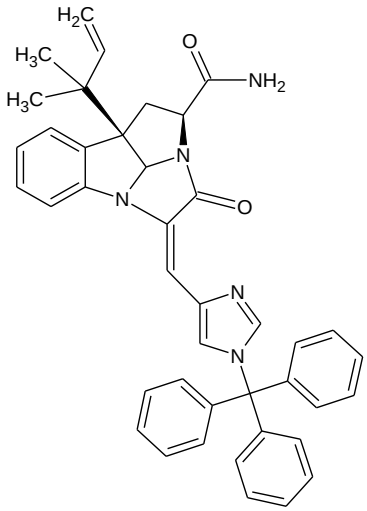
6. The final molecule with the customized radical labels should like the following:



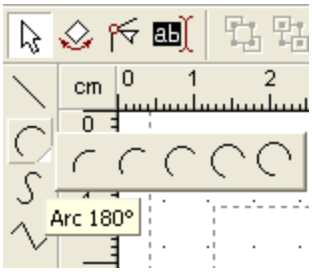
7. If you would like to apply this radical labeling style to any newly drawn radical labels, simply number your radicals and open the **Properties** dialog box (step 4). Then, apply the radical numbering style by choosing it in the **Current Style** drop-down and click **Apply**.

How to Draw Curved Arrows to Indicate What Nuclei are Coupling to Each Other

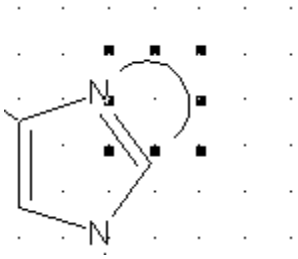
You can use ACD/ChemSketch to draw NMR correlations between nuclei, which typically appear as 'curved arrows'.



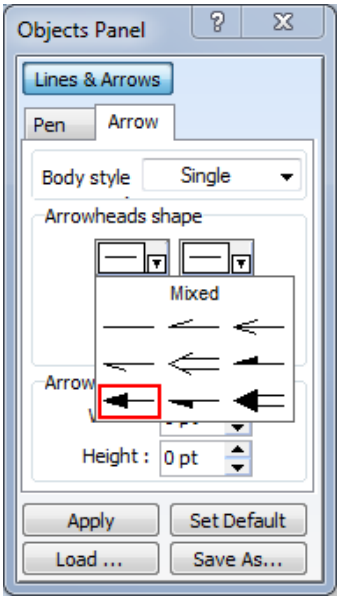
1. In the **ChemSketch** window, draw a structure.
2. To access the curved arrows, click **Draw**  to switch to the drawing shapes mode.
3. Along the left panel of ChemSketch, a new set of buttons will appear. Click the white triangle located on the bottom right corner of the **Arc** button to access more choices of arc angles.



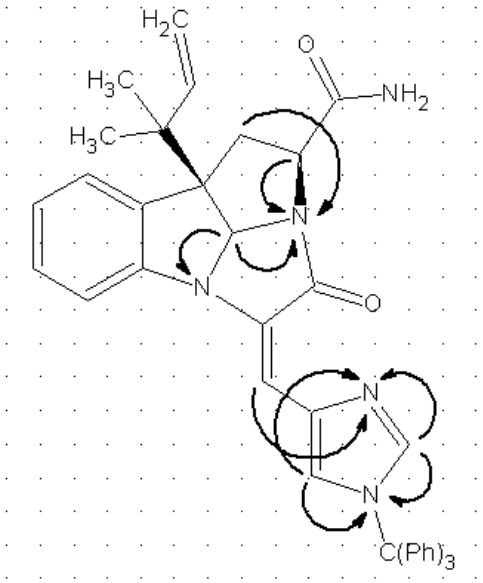
4. Select the **180º Arc**, point in the vicinity of an atom and click and drag to the second atom of interest. A nine-point boxed selection will appear around the arc.



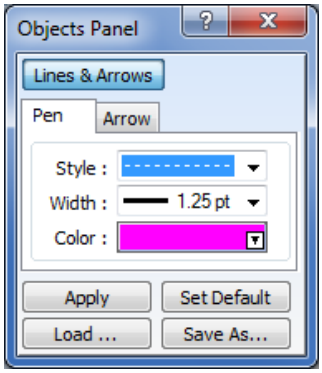
5. Double-click over the arc or from the **Tools** menu, choose **Update Object Style Panel** to open the **Object Panel** dialog box.
6. To apply the arrowhead, click the **Arrow** tab and from the **Arrowheads shape** box, click a shape.
7. Once the arrowhead has been selected, click **Apply** to set the arrowhead. If the arrow shape appears on the wrong end of the arc, simply click **Swap** to swap the position of the arrowhead, then click **Apply**.



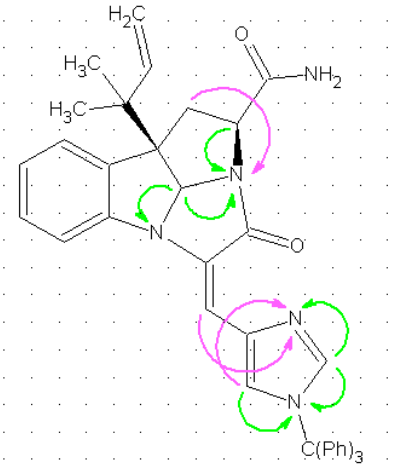
8. Repeat steps 4-7 to draw more curved arrows. To the right is a typical correlation map based on a $^{1}H,^{15}N$ HMBC experiment.



9. You can edit the **Style**, **Width** and **Color** of the arcs on the **Pen** tab. Change the **Style** to a dashed line to show ambiguous correlations. To differentiate between 2 and 3 bond correlations, apply a different **Color** to each. Click **Apply** to save your changes.



10. Below is a typical correlation map in color based on a $^{1}H,^{15}N$ HMBC. 2*J* and 3*J* correlations are shown in green and purple, respectively.



11. To add NMR information, on the left panel, click **Edit Text**. Then click the **ChemSketch pad** to enable textual information to be typed out.

> **Note** If the textual information needs further editing, on the toolbar, click **Edit Text**.

Below is a typical correlation map with chemical shifts from C.E. Hadden, D.J. Richard, M.M. Jouillie, G.E. Martin. (**2013**). Natural product synthesis with unnatural results: Characterization of a novel fused imidazolidinone tetrahydropyrroloindole ring system by long-range ^{1}H-^{15}N 2D-NMR. *J. Heterocyclic Chem*., *40*(2): 359–362.