Advanced Chemistry Development

Technical Note

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

ACD/ChemSketch 8.0

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Introduction

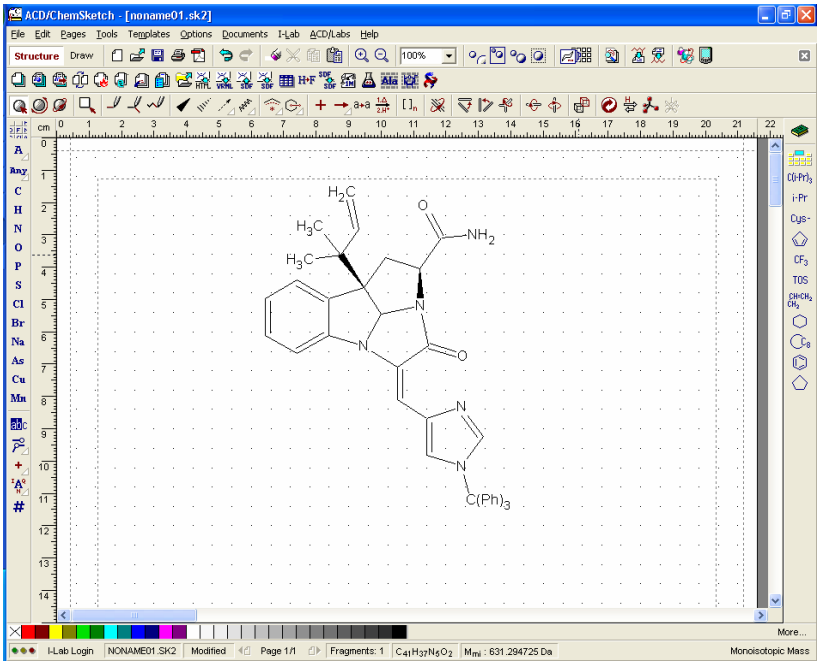
Traditionally, hand-drawn structures provide a quick representation to convey an idea(s) to other users. Through software drawing tools, users have the extra benefit of neatly drawn structures that are easy to read and easy to duplicate and maintain. The penultimate benefit is a report containing neatly drawn structures.

The following application note will illustrate the steps required to draw NMR correlations between nuclei that typically appear as 'curved arrows'. To perform this function, you will need ACD/ChemSketch [1].

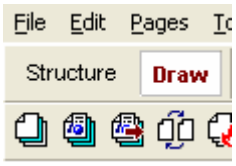
The Process

For the purposes of this example, we will not indicate how to draw structures. Information on how to draw structures is available in the *ACD/ChemSketch Tutorial*. The steps below will only demonstrate how to draw curved arrows with the appropriate textual chemical shift.

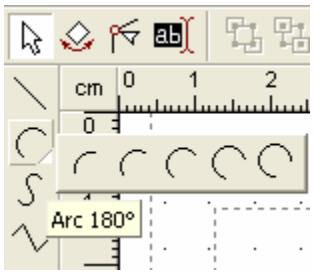
1. In the **ChemSketch** window, draw a structure.



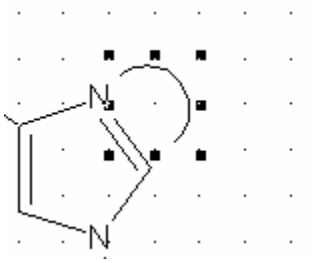
2. To access the curved arrows, click **Draw** to switch to the drawing shapes mode.



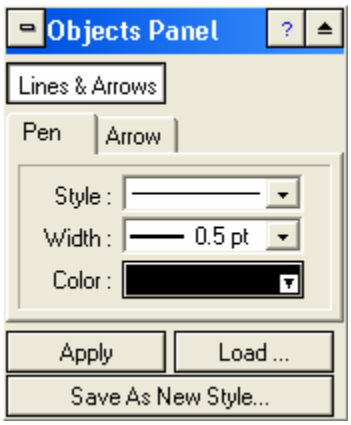
3. Along the left panel of ChemSketch, a new set of buttons will appear, one of which is the **Arc** button. Click the white triangle located on the bottom right corner of the **Arc** button to access more choices of arc angles.



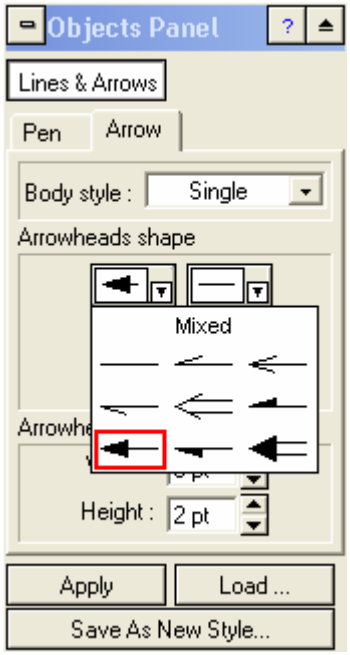
4. For the following screen shot, the **180º Arc** was selected. Point in the vicinity of an atom and click and hold, then drag to the second atom of interest. A nine-point boxed selection will appear around the arc.



5. Double-click over the arc or from the **Tools** menu, choose **Update Object Style Panel** to open the **Object Panel** dialog box.

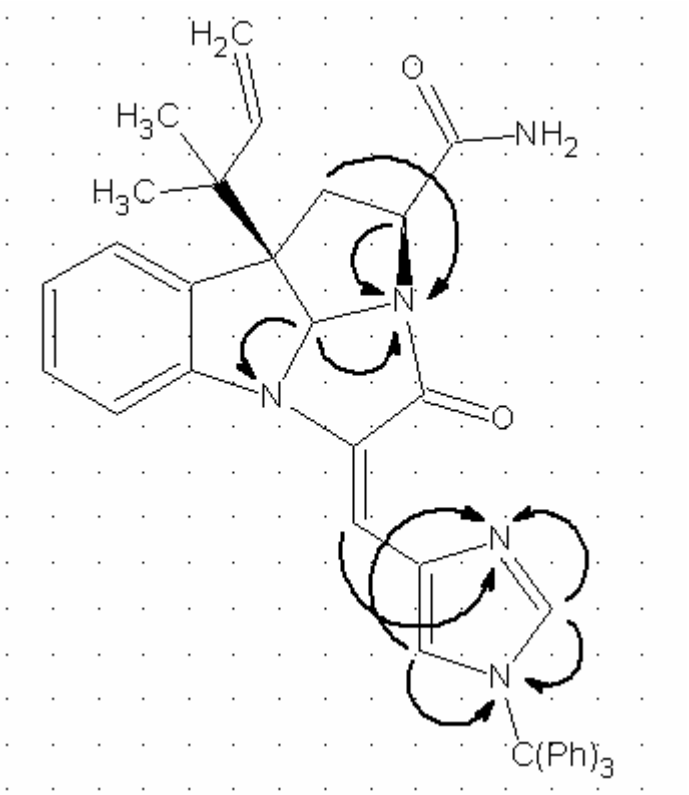


6. To apply the arrowhead, click the **Arrow** tab and from the **Arrowheads shape** box, click a shape.

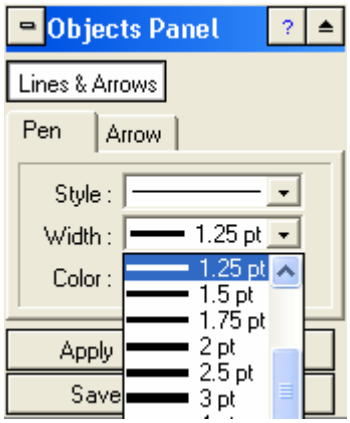


7. Once the arrowhead has been selected, click **Apply** to set the arrowhead. If the arrow shape appears on the wrong end of the arc, simply click **Swap** to swap the position of the arrowhead, then click **Apply**.

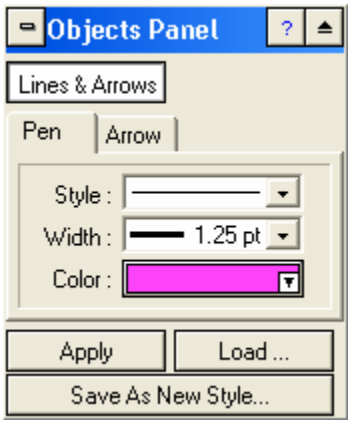
8. Repeat steps 4-7 to draw in more curved arrows. Below is a typical correlation map for a $^{1}H,^{15}N$ HMBC.



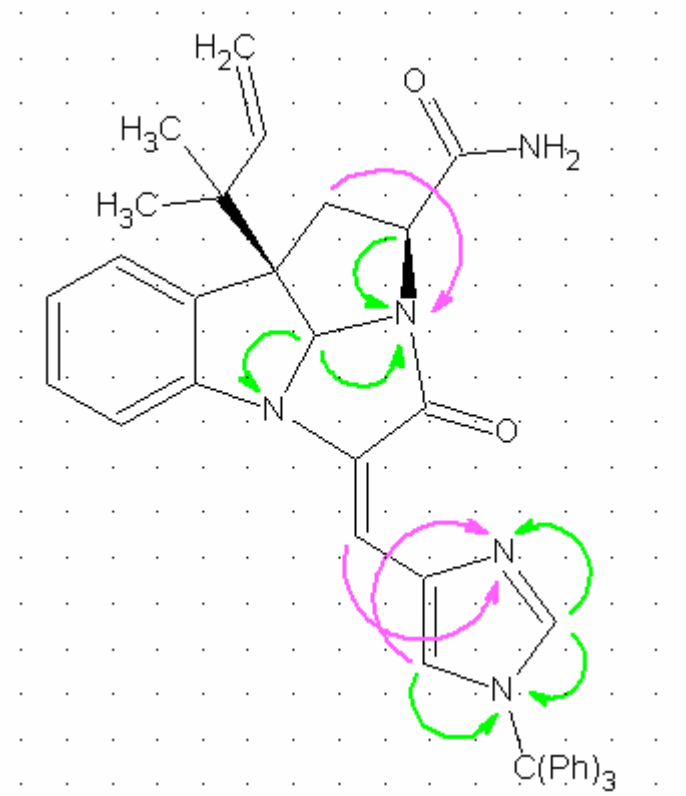
Note To apply a thicker line width to the arc, click the **Pen** tab, then in the **Width** box, click a value.



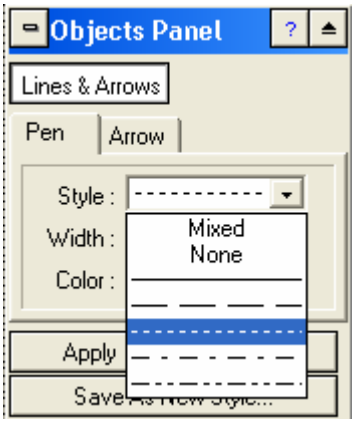
9. To apply color to the curved arrows—to differentiate between a 2 and 3-bond correlation—double-click on the curved arrow of interest, then from the **Color** box, click a color. Click **Apply**.



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



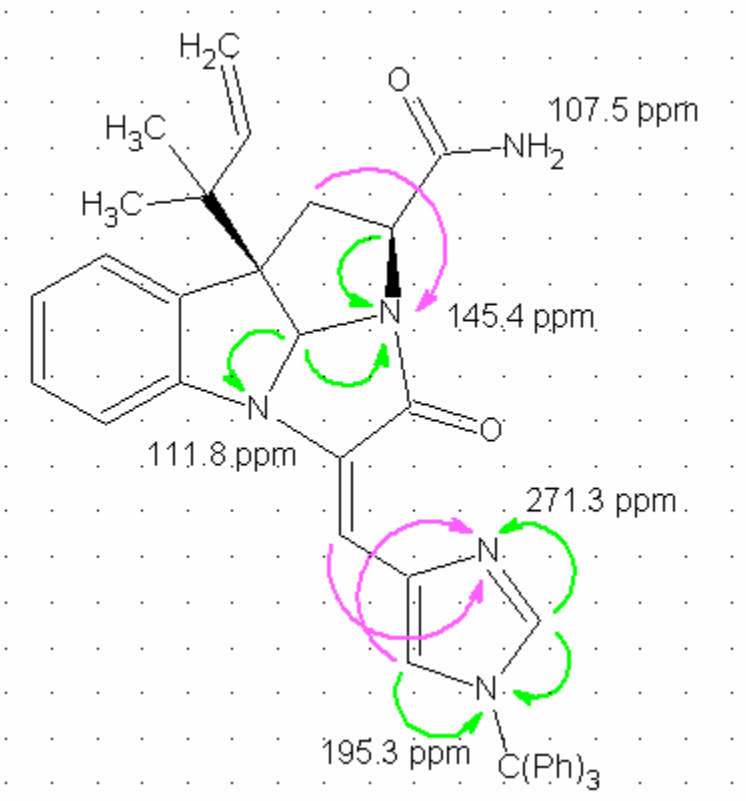
11. To add ambiguous correlations, double-click on the curved arrow of interest and change the **Style** in the **Objects Panel** dialog box, then click **Apply**.



12. 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**.

13. Below is a typical correlation map with chemical shifts from C.E. Hadden, D.J. Richard, M.M. Jouillie, G.E. Martin, *J. Heterocyclic Chem.*, 2003, **40**, 359.



References

1. ACD/ChemSketch. http://www.acdlabs.com/chemsketch/. January 14, 2005.