ChemSketch: Drawing Markush Structures

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Introduction

This guide is meant as a brief overview of the recommended steps for drawing Markush structures using ACD/ChemSketch. Additional documentation can be found by navigating to the **Help** menu then selecting **Reference Manual** and performing a search for the keyword "Markush".
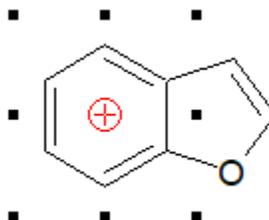
Tools

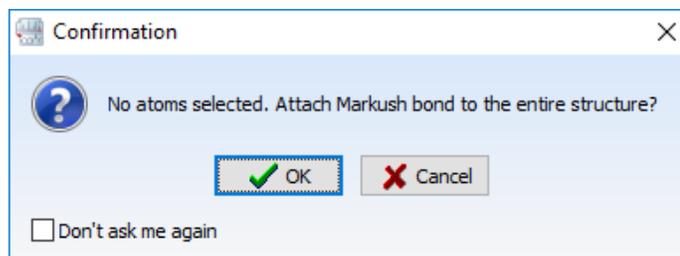The Markush Bond tool can be found in the upper toolbar.

Click the white triangle (highlighted in yellow) at the bottom corner of the icon to see other Markush drawing tools: Markush Bond with Shadow, Added or Removed Fragment, and Added or Removed Fragment with Shadow).
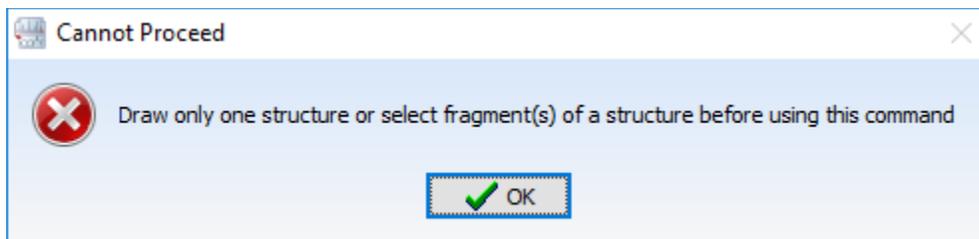
Inserting Markush Bonds

1. Begin by drawing a structure using the standard structure drawing tools. Select the part of the structure you want to connect the Markush bond to by using ( ) or ( ).
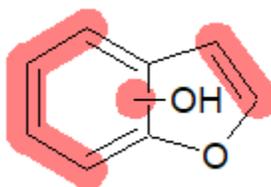

    Note: Clicking on any of the Markush Bond buttons without making a selection in your molecule first will lead to the following warning/question:
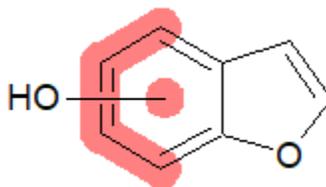

Note: If you have more than one drawn structure and you do not make a selection before choosing a Markush tool, you will receive the following instructions:

If you click **OK** the bond will be added to the entire structure. If you click **Cancel** the window will close and the Markush tool will be deactivated.
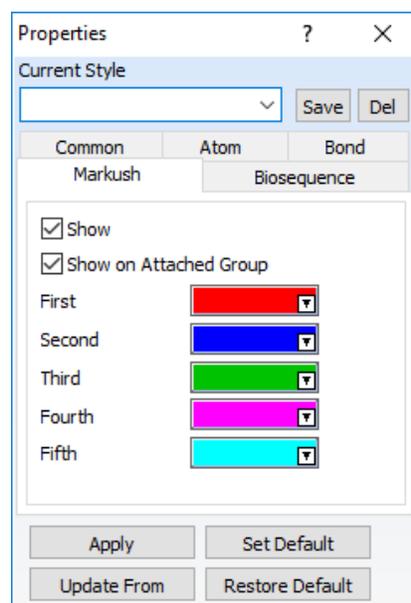

2. After selecting a portion of the molecule, click one of the Markush Bond buttons to insert the bond. You may click and drag on the substituent label (for example, the OH) to reposition the Markush bond on your structure.
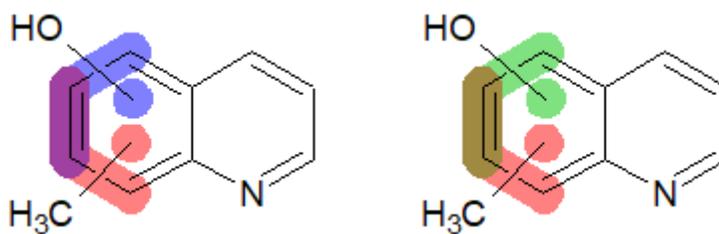

Note: The coloring for Markush shadows can be adjusted by going to **Options > Preferences** and editing the colors under the **Object Coloration** tab, or by right-clicking on the structure and selecting **Object Properties** and editing the colors under the **Markush** tab.
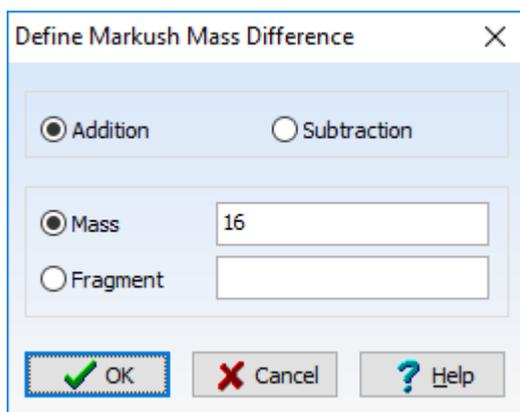
OR

Users should choose colors based on their preferences, taking into account the colors that are most clearly visible when printed and used in crossing shadows, as well as color blindness.

To avoid overlapping substituents, you may also move the entire substituent off the structure:

Note: If you select one of the Added or Removed Fragment Markush tools, the **Define Markush Mass Difference** dialog box will appear:
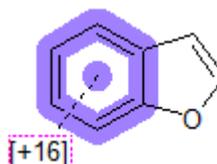
Input the necessary information and click **OK** to insert the mass difference or fragment.
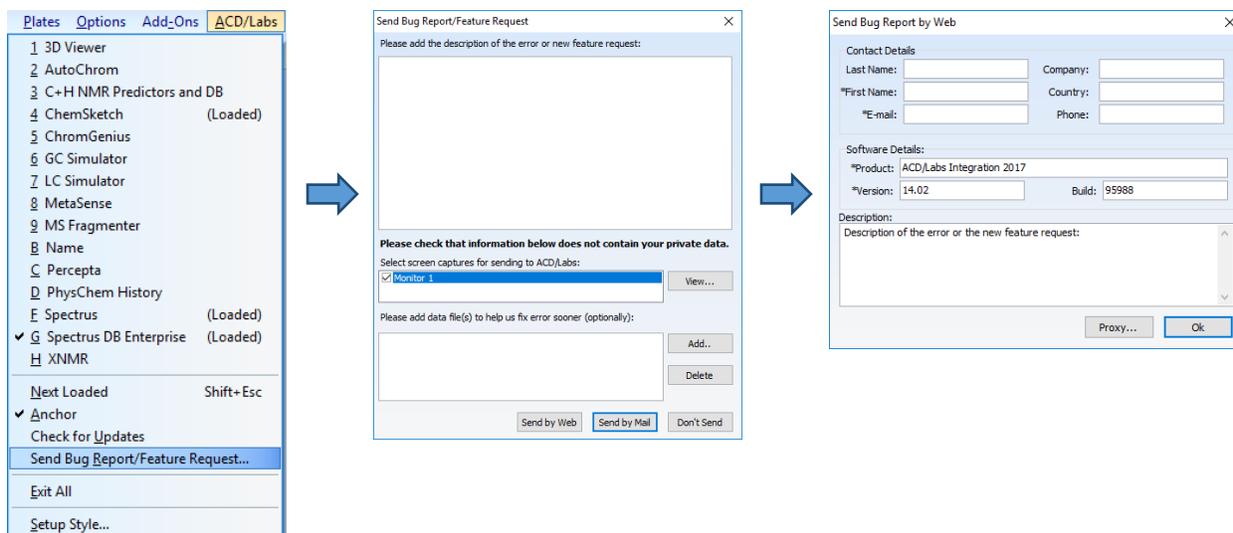

Search Tip

If you wish to perform a substructure search for structures with a Markush bond you should pay special attention to choosing atoms which you want to participate in Markush binding.

Conclusion

This guide is intended as a brief outline of the necessary steps for drawing Markush structures.

Please visit www.acdlabs.com for more details. If your software is on a computer connected to the internet, our technical support team can be easily contacted by selecting **Send Bug Report/Feature Request…** under the ACD/Labs menu, filling out the appropriate information and sending via Web or Mail.