

## ACD/ChemSketch: Drawing Polymers


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### Introduction


This guide will go through the polymer drawing tools in ACD/ChemSketch.

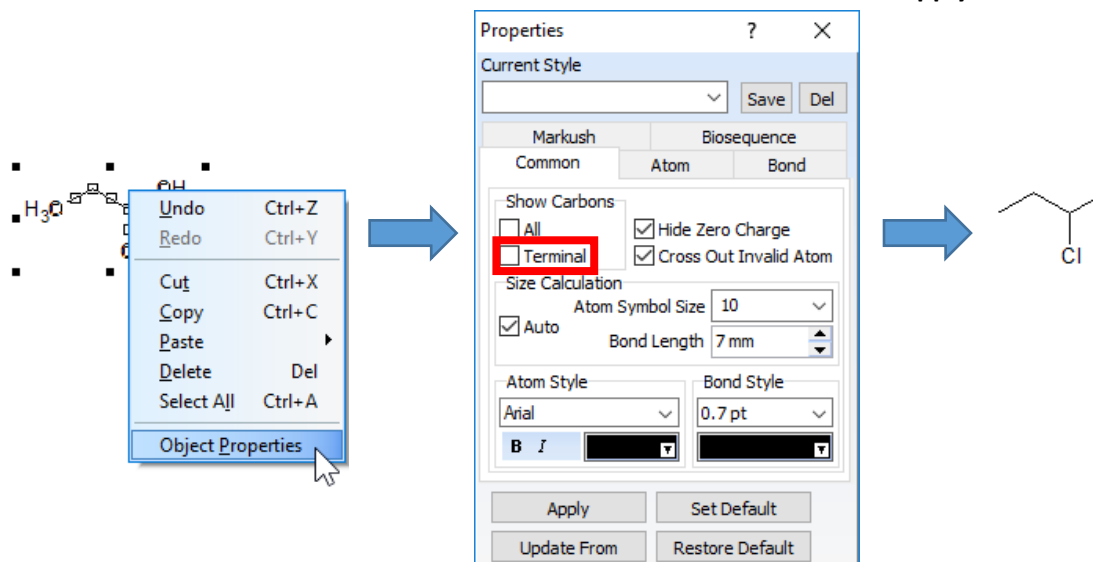
### Basic Drawing Tools

Begin by drawing a portion of your polymer, such as a repeat unit, using the simple drawing tools or templates as necessary.


**Note:** The draw chains () tool may be useful. Click, drag and release to draw a chain (length is defined by the cursor; holding "Ctrl" while using this tool will produce a linear chain).



It is sometimes desirable to leave undefined end groups. To adjust the display settings for terminal carbons, select the structure using the **Select** button () then right-click and select **Structure Properties** from the context menu. Turn off **Terminal Carbons** in the **Common** tab and click **Apply**.

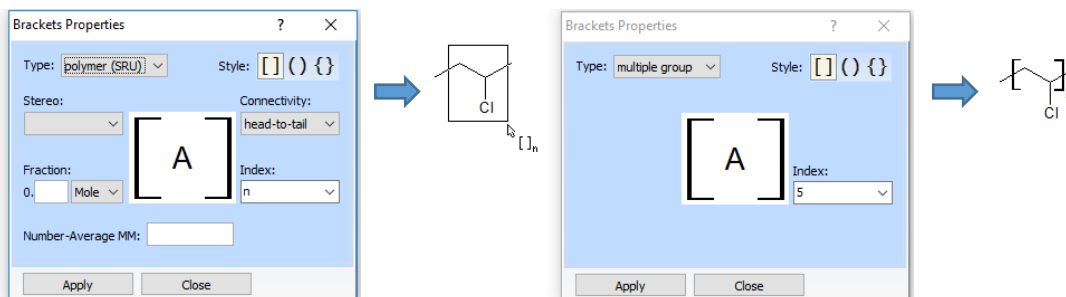


### Brackets Tool

The **Brackets Tool** in the top toolbar () allows you to draw brackets of a selected style and type around an existing structure. There are a number of possible combinations of styles and types; explore the drop-

down menus for each option to find the combination that suits your needs. You can also define mole/mass fraction and number-average MM.


**Note:** The Brackets Tool can be used to modify existing brackets. Open the tool and select the brackets you would like to modify, make changes, and then click **Apply**.

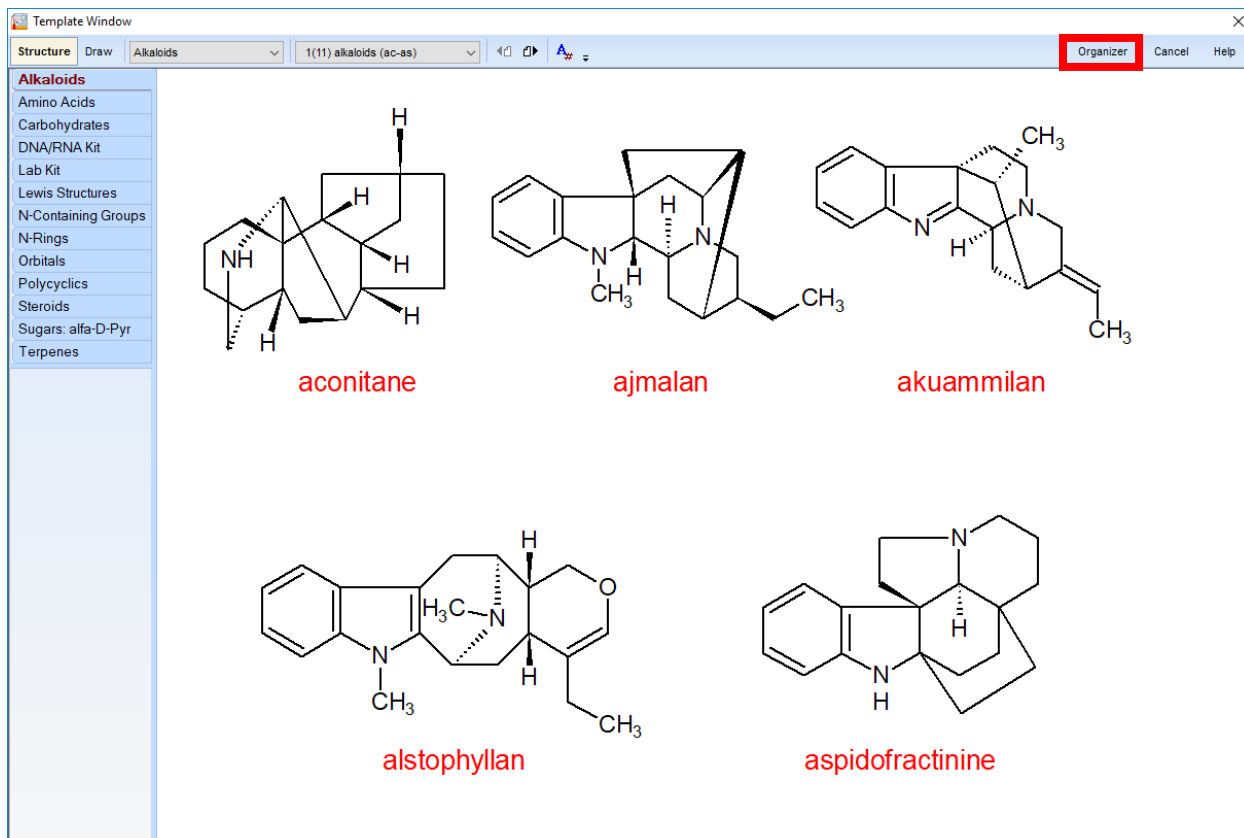


If the repeat unit of your polymer has been defined with a number, as shown above, the status bar at the bottom of the window will show the full molecular formula, FW, and  $M_{mi}$ .

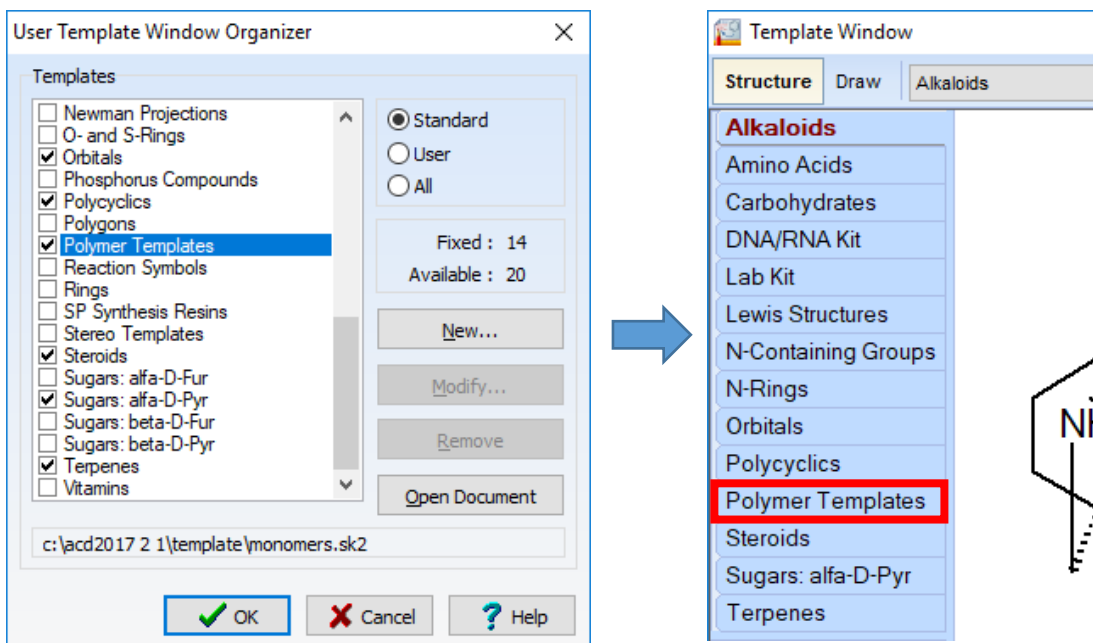
$C_{12}H_{21}Cl_5$  FW : 342.56014  $M_{mi}$  : 340.008589 Da

## Template Window

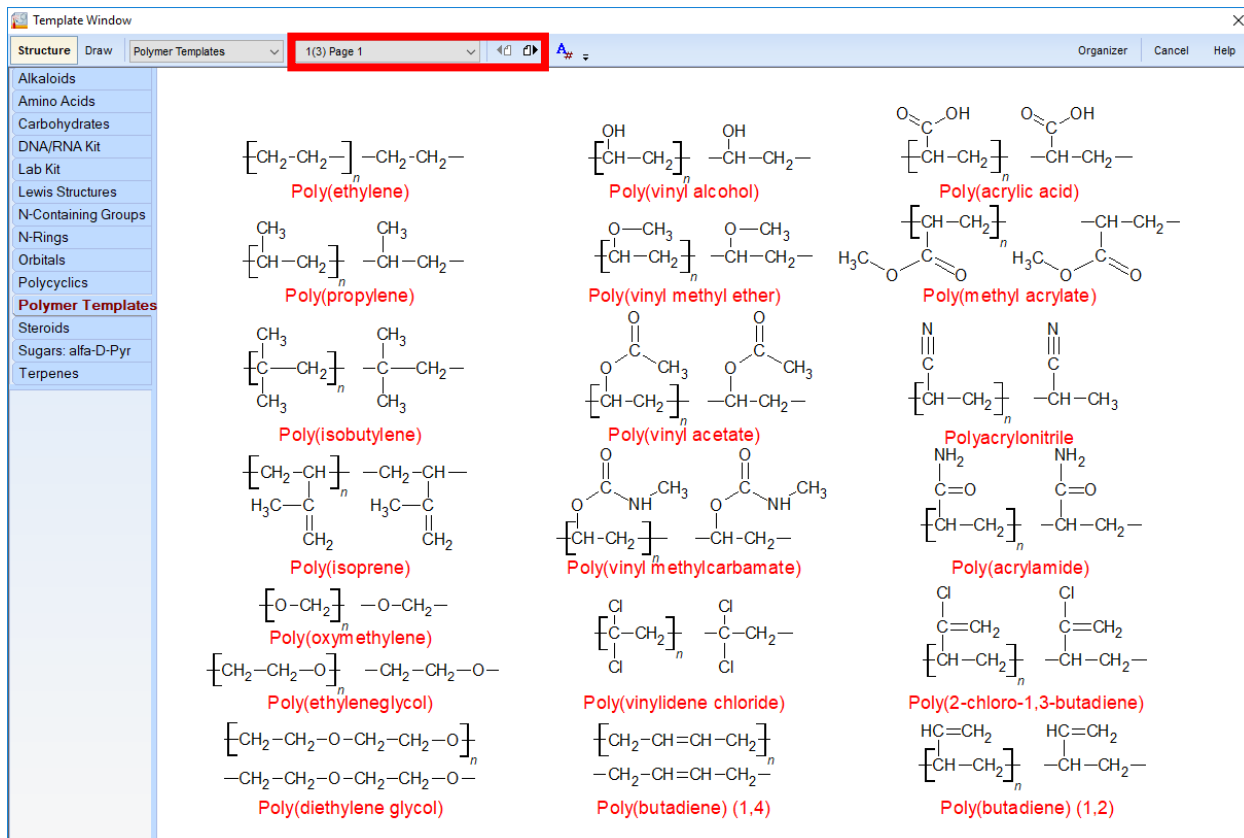
Access the polymer templates by clicking (  ) to open the Template Window or from the menu **Templates > Template Window**:



Go to **Organizer** and place a check mark next to **Polymer Templates**. It will appear in the Template Window list.




There are three pages of polymer templates included with the software. Use the arrow buttons or dropdown menu to navigate between pages.

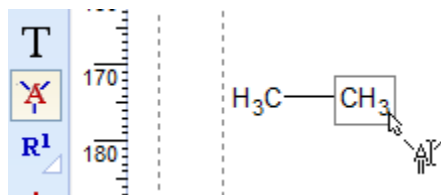


For each template entry, you have the option to choose the monomer or the pre-labeled polymer. Click on a structure to copy it to the clipboard and then click in the workspace to paste.

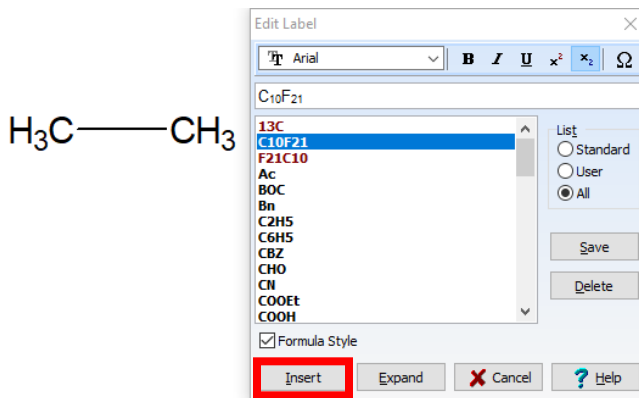
## Drawing Perfluoroalkanes

Follow these steps to draw the expanded structure of a perfluoroalkane:

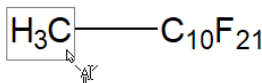
1. Draw ethane using the **Draw Normal** tool ()
2. Select the **Edit Atom Label** tool () then click on either carbon.




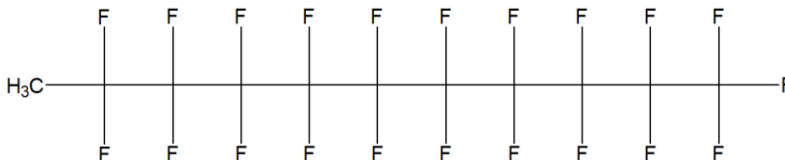
3. Type in the desired carbon/fluorine formula. The format must always indicate carbon first then fluorine, ex. C10F21, not F21C10 (even when editing the atom label on the left-hand side of the molecule).



4. Click **Insert** to change the label; repeat as necessary on the other end.



5. Select the structure using the **Select/Move** tool () then use the shortcut **Ctrl + Shift + F** to expand the shorthand formula.



**Note:** This function can also be accessed from the menu **Tools > Expand Shorthand Formulae** or the **Expand** button from the **Edit Label** dialog.

## Conclusion

This document describes the basic features of the software. For a more in-depth view of any of the individual features, please consult the software manual or **Help** menu.

Please also visit [www.acdlabs.com](http://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.

