ACD/ChemSketch: Biosequence Tools

Laura Zepeda
Advanced Chemistry Development, Inc.
Toronto, ON, Canada
www.acdlabs.com

Introduction

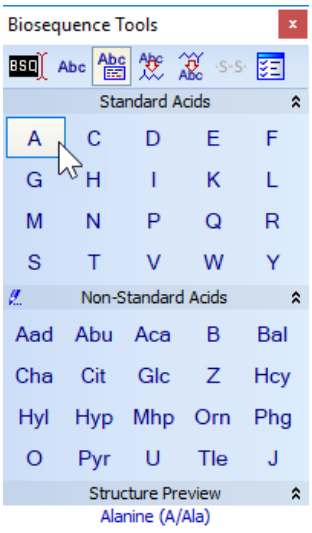
This guide demonstrates the Biosequence Tools that are available within ACD/ChemSketch.

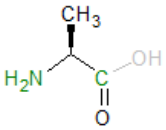
Accessing the Tools

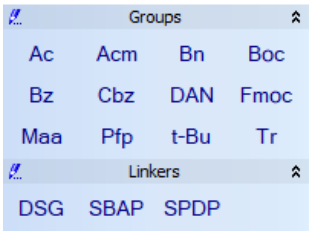
In order to work with the **Biosequence Tools** you must begin in **Structure** mode (

) then click the corresponding icon (

) in the drawing toolbar. This will open a new window in which you can find all of the biosequence tools.

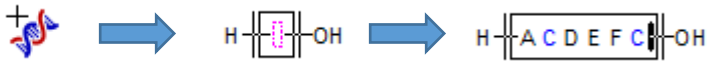




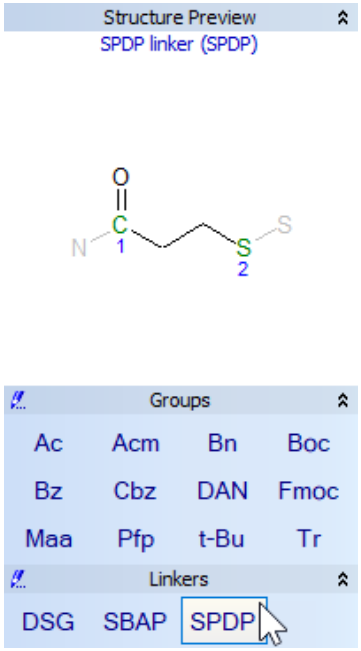


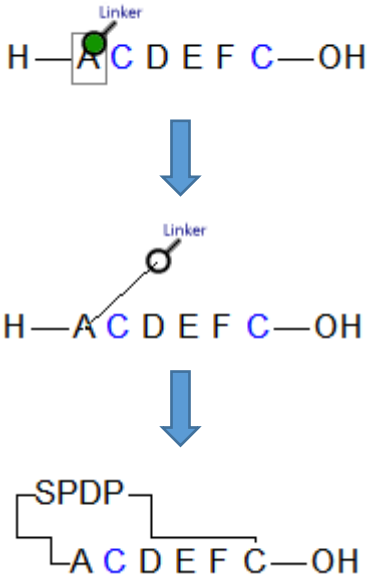
Using Biosequence Tools

Enable () to start generating a string of amino acids in your workspace. Click any acid to add it to your sequence. You can also click inside the workspace then use your keyboard to type out the single-letter notation for the acids in your sequence.



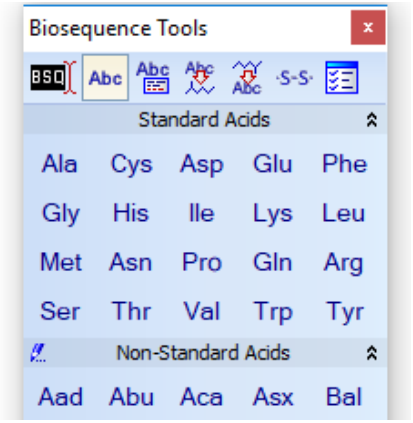
You can add **Groups** and **Linkers** to your sequence by selecting the desired group/linker and clicking on the appropriate acids. The mouse cursor will indicate whether an acid is appropriate for a selected group/linker by changing color as you hover over your sequence (red = incompatible, green = compatible), and the **Structure Preview** area of the **Biosequence Tools** window will indicate the requirements for each group/linker.



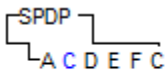


Click () to toggle three-letter notation on or off in your Biosequence Tools window and in a selected sequence.

H—Ala Cys Asp Glu Phe Cys—OH

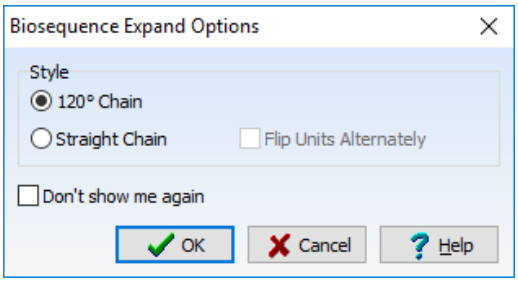


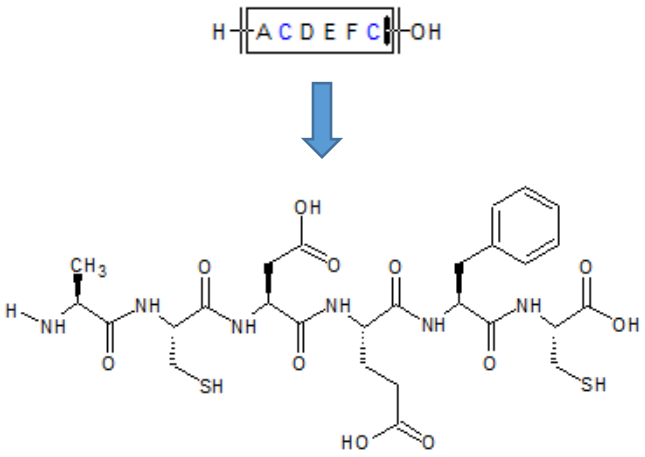
The ( ) icon allows you to toggle the sequence description on or off, listing the modifications and linkages present in your sequence.



Modified acids SPDP 1, 6;

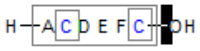
Convert a single-letter or three-letter sequence into a structure using this icon ( ).

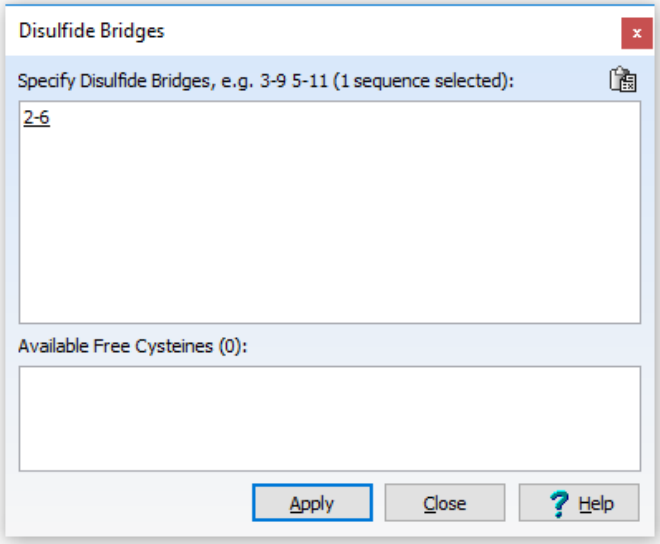




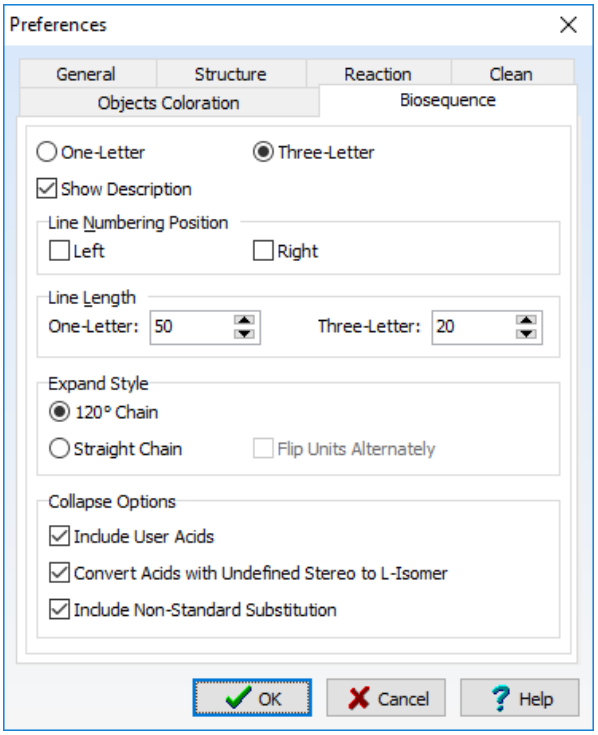
Revert to an abbreviated sequence using ( ).

When the necessary acids are present, you can insert a disulfide link using this button (). You can then specify the cysteine residues you would like to link (available ones will appear in the "Available Free Cysteines" box).



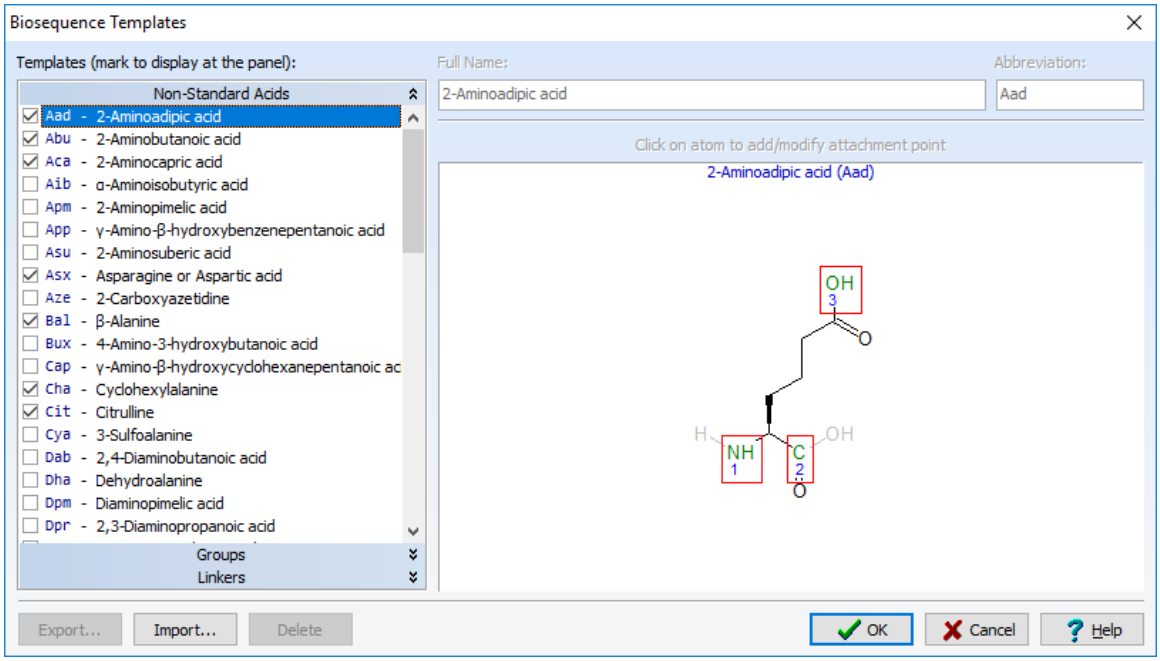


Adjust your biosequence preferences using ().

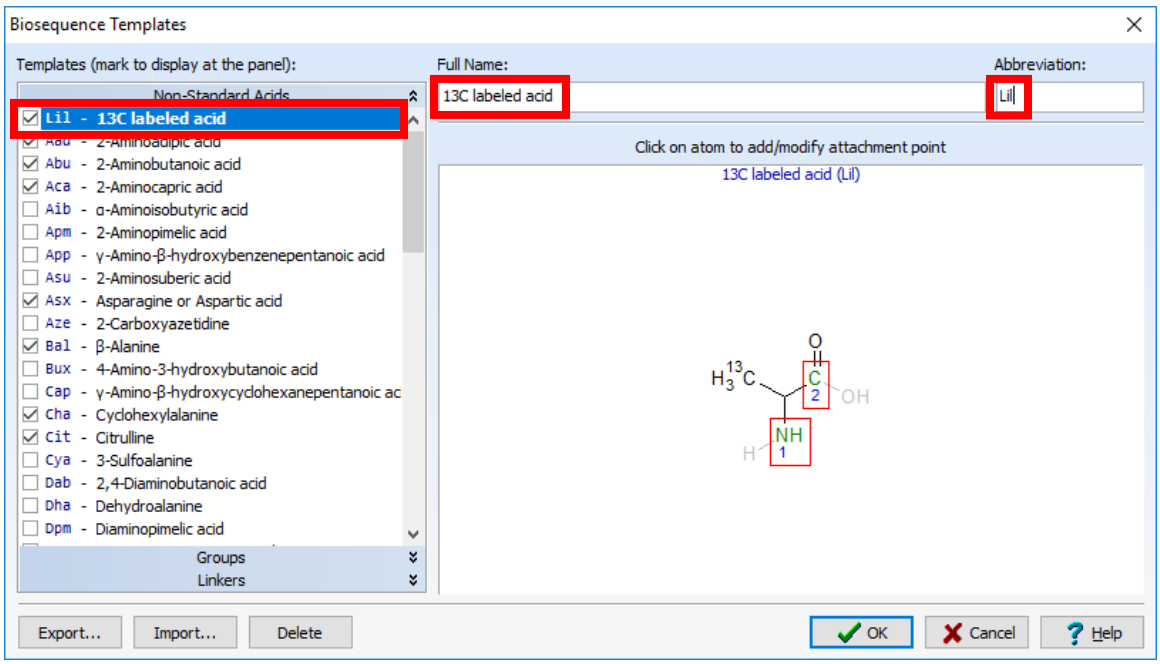


Editing Acids, Groups, and Linkers

You may change the default Non-Standard Acids, Groups and Linkers that are displayed in the **Biosequence Tools** window by clicking on the ( ) icon at the top left corner of each section.



A user template may be added by clicking **Import** (select an existing *.sk2 file) or by drawing the template structure in the ChemSketch workspace and selecting it. When you do this, the ( ) icon changes to ( ) and you may click this new icon to add the template to the appropriate section.



Conclusion

This guide is a quick introduction to the use of Biosequence Tools in ChemSketch. 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 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.