

ACD/Labs ChemSketch (Version 7.0)

Technical Note

***Preparing Structures for Literature Article
Submissions***

Written by: Rhiannon Jones

Advanced Chemistry Development, Inc.

Copyright © 1994–2002 Advanced Chemistry Development, Inc. All rights reserved.

ACD/Labs is a trademark of Advanced Chemistry Development, Inc.

All the other trademarks mentioned within this Manual are the property of their respective owners.

All trademarks are acknowledged.

Information in this document is subject to change without notice and is provided "as is" with no warranty. Advanced Chemistry Development, Inc., makes no warranty of any kind with regard to this material, including, but not limited to, the implied warranties of merchantability and fitness for a particular purpose. Advanced Chemistry Development, Inc., shall not be liable for errors contained herein or for any direct, indirect, special, incidental, or consequential damages in connection with the use of this material.



1. Introduction

Every journal has its' own editorial style, and chemical structures which are included in literary articles must conform to specific drawing styles. The Royal Society of Chemistry provides guidelines for chemical structures at its webpage (<http://www.rsc.org/is/journals/illustrations/illustrations.htm>) and while ACD/ChemSketch is not explicitly listed at present, the RSC has accepted the request to list our product and will be updating the webpage shortly.

The American Chemical Society outlines on its Paragon webpage that chemical structures need to be prepared according to specific guidelines. These parameters are specifically for ChemDraw but authors can use other drawing packages provided these parameters are adapted to their systems. (https://paragon.acs.org/paragon/application?pageid=content&mid=ag_preparing_illustrations.html&parentid=authorchecklist&headername=Preparing%20Graphics). This document confirms that such criteria can be met and already a series of publications HAVE been published in ACS journals using ACD/ChemSketch as the drawing package (see for example those articles listed at http://www.acdlabs.com/products/spec_lab/complex_tasks/str_elucidator/reviews.html#Structure_Elucidator-Based_Peer-Reviewed_Articles).

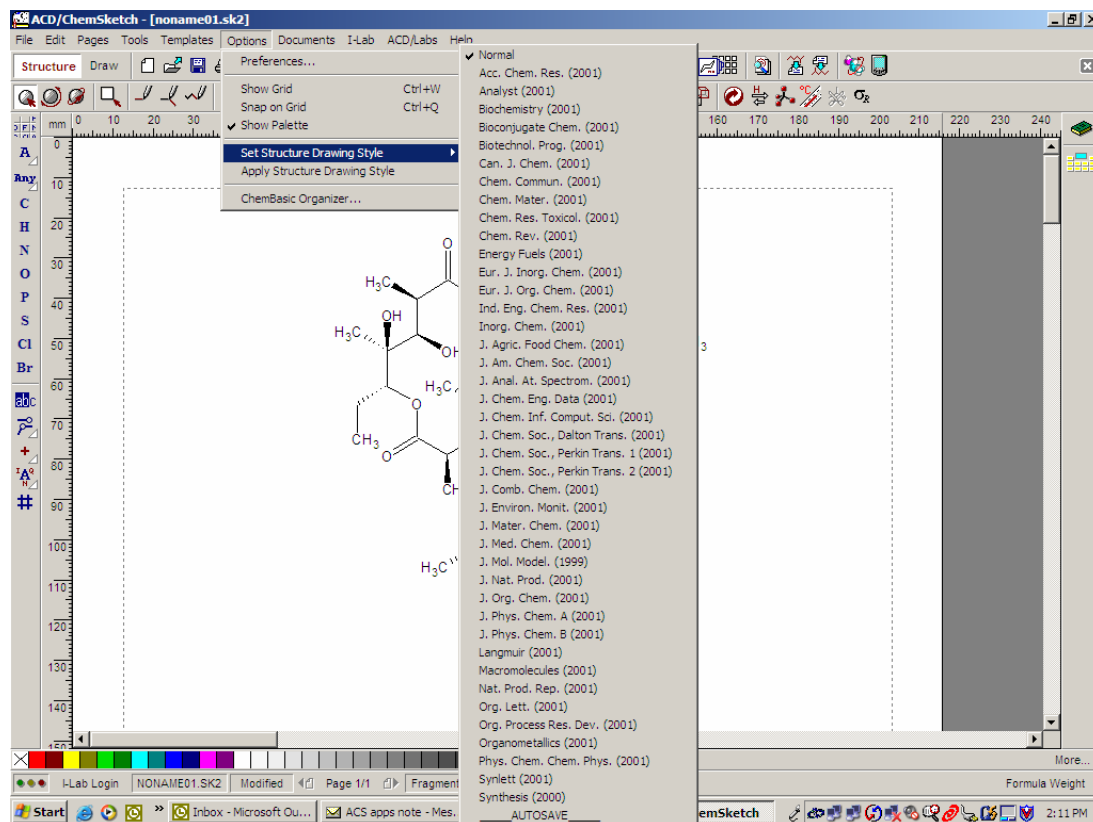
Rather than spending time manually changing each setting one by one, it is possible to easily select various journal styles within ACD/ChemSketch. This technical note will tell you how to apply the style you require to your structure.

2. The Process

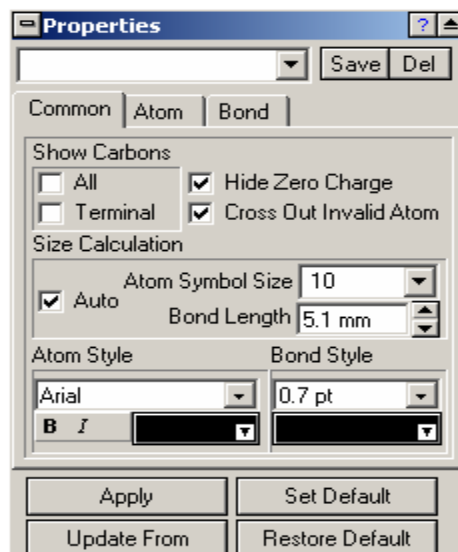
1. Open ChemSketch, and draw the structure of interest.
2. If the structure has been drawn freehand, it may need to be tidied up. Highlight the whole structure using the **Select/Move** button . Now click **Clean Structure** . This will unify all bond angles and lengths for your structure.

2.1 Selecting a Journal Style

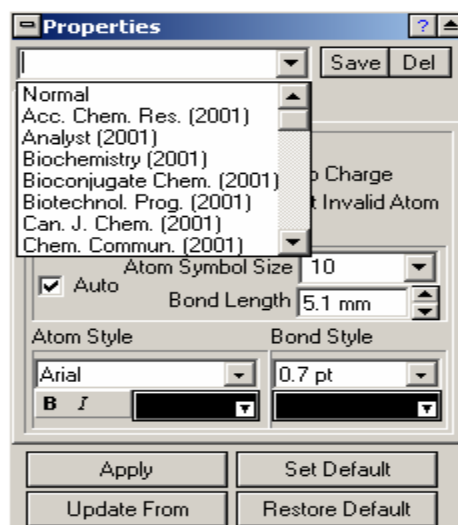
1. From the **Options** menu, point to **Set Structure Drawing Style**, and then choose the preferred drawing style (as indicated below):



2. Alternatively, you can double-click with the left mouse button on the structure. This will open the **Properties** window as follows:



3. Use the top pull down menu to select the journal style:



4. This will change drawing properties such as text type, bond length, and width in accordance with the specifications of each individual journal. Click **Apply** and the structure style should now change according to these settings. You can select this style to be the default style for future structures by clicking **Set Default**.

2.2 ACS Settings

Many journals specify that structures must conform to the American Chemical Society guidelines. Previously these guidelines stated that ISIS or ChemDraw had to be used, but now any drawing program can be used as long as it matches the appearance produced by these packages.

The settings are as follows:

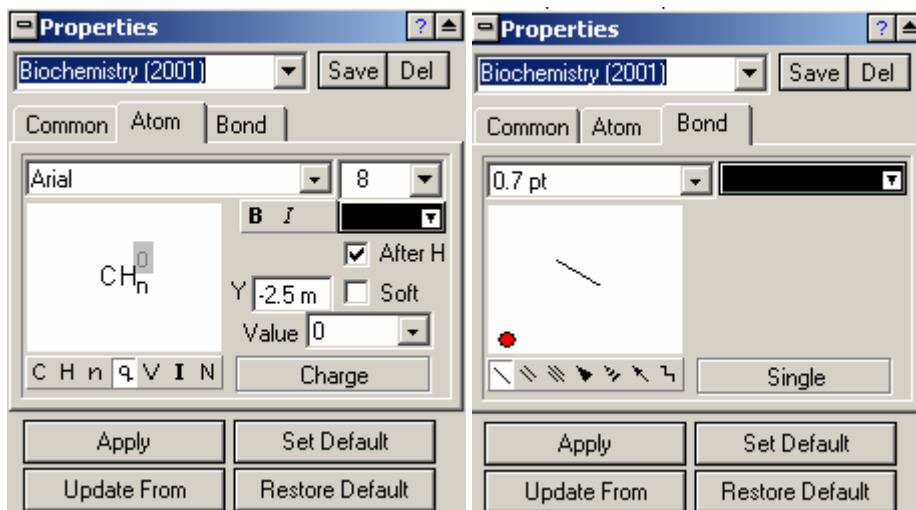
- Chain angle 120 degrees
- Bond spacing 18% of the length

- Fixed length 14.4 pt (0.2 in.)
- Bold width 2.0 pt (0.0278 in.)
- Line width 0.6 pt (0.0083 in.)
- Margin width 1.6 pt (0.0222 in.)
- Hash spacing 2.5 pt (0.0345 in.)

This style is one of the options in the list and has been saved as J. Am. Chem. Soc. (2001). There are other literary styles available such as Journal of Organic Chemistry and European Journal of Inorganic Chemistry, among many others.

2.3 Creating a New Journal Style

1. If you would like to create your own style, type your desired style name in the top blank line and click **Save**. This style will now be available as an option in the pull down list. It can be deleted from the list at any time by highlighting that name and clicking **Del**.
2. There are three tabs to choose from: Common, Atom, and Bond.



Properties such as numbering, valency, and charge can be changed under **Atom**. Under **Bond**, properties such as width of lines and the spacing between the lines in stereo wedges can be altered.