

## Primer for ChemSketch

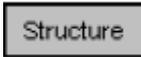
ACD/ChemSketch  
Version 10

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### Introduction

The following document provides a basic guideline to the operation of ACD/ChemSketch<sup>1</sup>, and is designed as a practical introduction for new users to become confident in utilizing the application to document chemical information.

### Modes of the Application

There are two modes to ACD/ChemSketch, namely **Structure**  and **Draw** . **Structure** mode enables you to draw chemical molecules, while in **Draw** mode you can create and edit graphical objects. Switching between the modes will cause the toolbars on the left, top, and right of the drawing space to change accordingly.

### Drawing Simple Molecules

Upon startup, the **Draw Normal** mode  and **Carbon**  are automatically selected. By clicking and dragging the cursor in the window, C-C bonds are created. Clicking on a carbon atom produces a branched structure, e.g., isopropyl. The software keeps track of the valency of the atoms and alerts you if this is exceeded by crossing out the atom. By repeatedly clicking on a bond, the saturation will cycle from single bond to double bond to triple bond.

Additional bond types can be selected by clicking **Up Stereo Bonds** , **Down Stereo Bonds**  or **Undefined Stereo Bonds** . By clicking on the white triangle in the lower right corner of an icon (if present), additional icons become available.

It is recommended that the entire skeleton of the compounds be drawn in carbon and then populated with heteroatoms as the last step. The change can be made by selecting a heteroatom from the element list in the left toolbar and clicking on an atom in the structure to replace it.

The element list can be customized by clicking **Periodic Table** .

The valence, charge, and isotope can be modified by clicking **Atom Properties**  and selecting the atom of interest.

ChemSketch interfaces directly with **MDL ISIS/Draw**, and supports direct cut and paste operations between the applications.

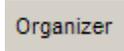
The **Table of Radicals**  contains the most common predefined radicals for chemical drawing, including carbon **rings**, carbon-based **side chains**, **functional groups**, protecting groups, and amino acids. By clicking on an entry in the table, the radical is selected and appears as a button on the right toolbar for future use.

The **Template window**  contains structures of complex molecules or illustrations, which would be otherwise difficult or time-consuming to draw by hand. The simplest way to navigate through the existing templates is to use the drop down boxes to select a template and then view the relevant pages relating to that template, i.e., in the example below there are 11 pages of structures for the alkaloid template



Upon clicking on an atom of a structure in the template window, you are transferred to the ChemSketch window where the structure can be positioned and edited.

Existing ChemSketch documents can be added in as new templates by clicking **Organizer**

**Organizer**  and then clicking **New** from the popup window.

**Note** It may be necessary to de-select some of the currently displayed templates before a new template can be added.

The **Dictionary**  contains ca. 157,000 entries pertaining to commonly encountered organic molecules, agrochemicals, and pharmaceutical agents. The database can be searched by typing part of the trivial name, CAS number, or IUPAC name in the **Quick Search** window.



By clicking **OK**, the structure is transferred to the ChemSketch window where it can be positioned. If a structure is already present in the ChemSketch window when the Dictionary icon is clicked, the software offers you the opportunity to search for that structure within the database.

Drawing reactions requires the use of the **Reaction Arrow**  and **Reaction Plus**  icons. By clicking on the white triangle of the reaction arrow icon, additional options become available. If additional annotation is required, e.g., reagent, catalyst, or temperature, select the **Reaction**

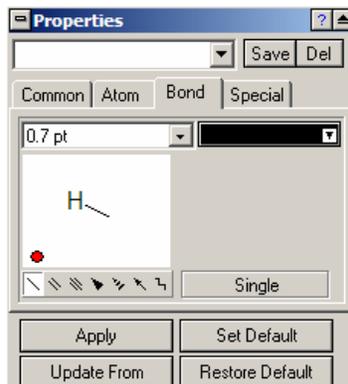
**Arrow Labeling** tool  and click on the reaction arrow.

## Cleaning and Customizing the Structure

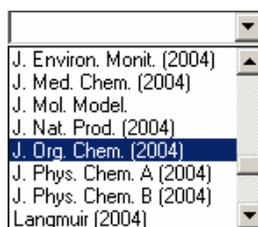
If you have made an error in drawing, click **Erase**  and click on the atom to remove it.

The bond lengths and bond angle can be standardized by clicking on **Clean Structure** .

By double clicking on any bond in the structure, you can edit the properties and drawing style:



Alternatively, you can choose from pre-defined drawing styles based on literature precedent from the drop-down list:



## Selecting and Moving Molecules

Depending on the mode of the **Lasso tool** , structures can be selected by clicking

**Select/Move**  and drawing a box or circle around the structure of interest (either the full structure or part of a structure can be selected). As a shortcut, if you position the cursor anywhere near a molecule and click once, the nearest molecule will be selected.

Once selected, the molecules appear with boxes over the atoms and bonds, i.e.,  $\text{H}_3\text{C}=\text{CH}_3$ .

The molecules can be repositioned by moving the cursor over the bond such that the boxes become filled, i.e.,  $\text{H}_3\text{C}=\text{CH}_3$ , and clicking and dragging. Clone structures can be made by pressing and holding SHIFT before clicking and dragging.

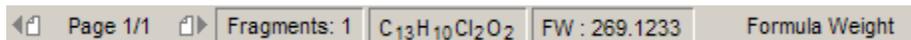
Different views can be obtained by selecting the **2D Rotate Tool**  or **3D Rotate Tool** .

Once a structure is selected, the options of **Cut** , **Copy** , and **Paste**  are available for use.

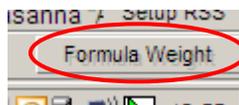
## Tools and Features

### Calculated Properties

The status bar reflects the number of compounds present (Fragment) and their combined properties.



The calculated property can be changed by clicking **Formula Weight** in the far right corner:



The calculated properties can be inserted into the ChemSketch window as a text field; on the **Tools** menu, point to **Calculate**, and choose the desired property.

### IUPAC Naming, SMILES and InCHI Code

By selecting a structure and clicking on **Generate Name for Structure** , the IUPAC name is generated as a text field underneath the structure. The algorithm is restricted to 50 atoms (excluding H) and 3 rings (a [commercial application](#) is available for more complex structures).

To access additional naming features (including SMILES and InCHI code), on the **Tools** menu, point to **Generate**, and choose the desired feature.

### Tautomerisation

To check for the presence of **tautomers** within a molecule, click **Check for Tautomeric Forms**

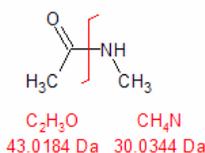


once a structure has been selected. If the structure contains possible tautomeric forms, you are given the option to scroll through the structures and may opt to replace the original structure.

### Mass Spec Fragment Calculator

When reviewing mass spec data, it is often useful to calculate the potential fragment losses within a molecule. By clicking on a single bond within a structure to select it and then clicking **Mass**

**Spec Scissors** , the application draws in the Formula and MW of the two halves (golden pairs) of the molecule:

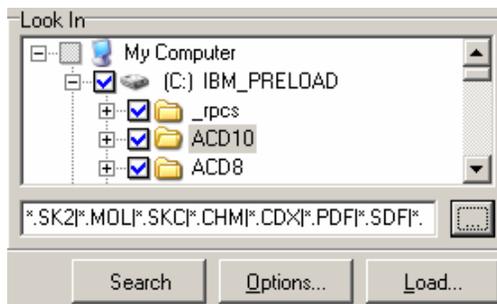


### Search for Structure

The **Search for Structure**  tool enables you to execute exact, sub-structure, or similarity searches for structures within various file types, e.g., ChemSketch, ISIS/Draw, or ChemDraw™

files, molfiles, or SDfiles, as well as any files which may have been embedded in other applications, e.g., Microsoft Word, Excel, or PowerPoint.

By drawing a structure and clicking on the icon, a new window opens which allows you to define the region of the network to search, the types of files to search and options for searching:



## Search Online Databases Based on Structure (Pubchem & EMOolecules)

As a service to our customers, we offer the capability to directly query the on-line databases of **Pubchem**  and **EMolecules**  from within the ChemSketch window.

By drawing a structure and clicking on the relevant database icon, the search results can either be displayed in the ChemSketch or Internet browser window.

**Note** The search requires an active connection to the Internet and is not secure. For this reason, we do not propose that confidential structures be used.

## Conclusion

The document describes the basic key features of the software. Many additional features and options are available—for a more detailed description of these, please consult the *ACD/ChemSketch Tutorial* (CHEMSK\_T.PDF) and *Reference Manual* (CHEMSK\_R.PDF).

Please also visit our website ([www.acdlabs.com](http://www.acdlabs.com)) for more details, updates, and to download free plug-ins for ChemSketch.

## References

1. ACD/ChemSketch. [www.acdlabs.com/chemsketch/](http://www.acdlabs.com/chemsketch/) Advanced Chemistry Development, Inc., Toronto, ON, Canada. 21 February 2007.