

## ACD/ChemSketch for Mass Spectrometrists

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### Introduction

This document outlines functions of ACD/ChemSketch that are useful for mass spectrometrists including calculating properties for a structure or fragment, displaying properties on the status bar, adding a charge to a structure, drawing Markush structures, and templates.

### Structure Mode vs. Draw Mode

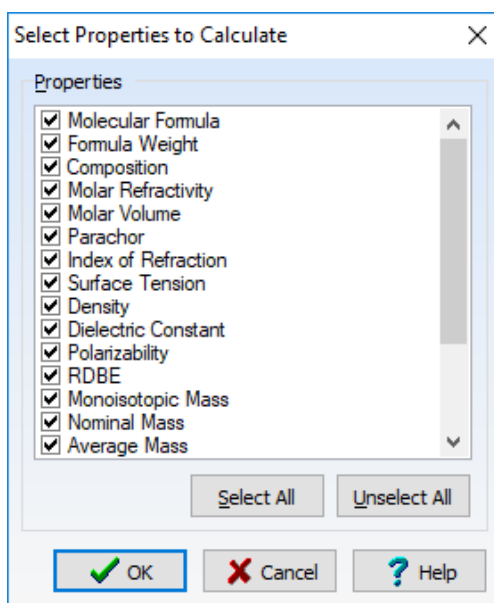
There are two modes available in ACD/ChemSketch. Structure mode for drawing chemical structures and calculating their properties. Draw mode for text and graphics. The menus and toolbars change when switching between modes.

To switch between these modes use the buttons   on the general toolbar.

### Calculating Selected Properties

You may find that you calculate a group of chemical structure properties often, e.g., Molecular Formula and Monoisotopic Mass. It can be useful to calculate all of these properties at once.

In structure mode, draw or open a structure in the workspace window. On the **Tools** menu, point to **Calculate**, and then choose **Select Properties to Calculate**. In the **Select Properties to Calculate** dialog box, select the properties that you want displayed, such as monoisotopic mass, and click **OK**.



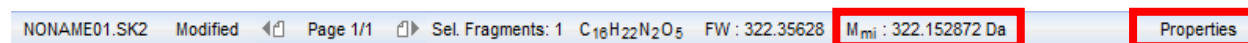
Go back to the **Tools** menu, point to **Calculate** and then choose **Selected Properties**. The **Calculation Results** dialog box appears with only the selected properties calculated.

The screenshot shows the ACD/ChemSketch interface with a chemical structure of a substituted benzamide derivative. The structure is displayed in the workspace, and a list of calculated properties is shown to its right. The properties include molecular formula, formula weight, composition, molar refractivity, molar volume, parachor, index of refraction, surface tension, density, dielectric constant, polarizability, RDBE, and various mass values (monoisotopic, nominal, average, and M+/-).

Molecular Formula:	C <sub>16</sub> H <sub>22</sub> N <sub>2</sub> O <sub>5</sub>
Formula Weight:	322.35628
Composition:	C (59.61%) H (6.88%) N (8.69%) O (24.82%)
Molar Refractivity:	85.00 ± 0.3 cm <sup>3</sup>
Molar Volume:	250.6 ± 3.0 cm <sup>3</sup>
Parachor:	692.6 ± 4.0 cm <sup>3</sup>
Index of Refraction:	1.593 ± 0.02
Surface Tension:	58.2 ± 3.0 dyne/cm
Density:	1.285 ± 0.06 g/cm <sup>3</sup>
Dielectric Constant:	Not available
Polarizability:	33.69 ± 0.5 · 10 <sup>-24</sup> cm <sup>3</sup>
RDBE:	7
Monoisotopic Mass:	322.152872 Da
Nominal Mass:	322 Da
Average Mass:	322.3563 Da
M+:	322.152323 Da
M-:	322.15342 Da
[M+H] <sup>+</sup> :	323.160148 Da
[M+H] <sup>-</sup> :	323.161245 Da
[M-H] <sup>+</sup> :	321.144498 Da
[M-H] <sup>-</sup> :	321.145595 Da

## Displaying the Monoisotopic Mass on the Status Bar


In structure mode, draw or open a structure in the workspace window. To view the monoisotopic mass for the structure selected in the workspace on the status bar, click on the field on the far right of the status bar ( **Properties** ). The default option is Formula Weight. A menu appears to select the desired property to be displayed. Select **Monoisotopic Mass**.



If a structure is not selected in the workspace, the property is calculated for all displayed structures.





## Calculating Monoisotopic Mass for a Fragment – MS Scissors

In Structure mode, draw or open a structure in the ChemSketch window. Select a bond to cut. You break a cyclic structure by holding down the SHIFT key, and selecting the cyclic bonds to cleave.

Select the bond(s) to break. On the Structure toolbar, click **MassSpec Scissors** . With the settings from the last section, you will be able to view the monoisotopic mass of each fragment in the status bar by selecting the individual fragments.

## Adding a Charge or a Radical to a Structure



In structure mode, draw or open a structure in the workspace window.



On the Atoms toolbar, click the bottom right triangle of **Increment (+) Charge** () to expand more buttons. Click the **Increment (+) Charge** () , **Decrement (-) Charge** () , or one of the **Radical** buttons () and then click on the atom in the structure to add the charge or radical to it.

## Markush Structures



Sometimes, it is not possible to fully elucidate a structure with mass spectrometry, but it is useful to keep track of the partially elucidated structure. Markush representations allow you to indicate multiple sites of attachment for a particular fragment or mass value.

In Structure mode, draw or open a structure. On the structure, select the atom(s) or bond(s) which indicate the possible sites of attachment. Hold down the SHIFT key to select multiple sites.

Mouse over the **Markush Bond** () button, and click the white triangle to show all types of Markush structures () . Depending on the type of Markush bond you want to apply, perform one of the following steps:

1. To display the structural fragments, on the Structure toolbar, click either **Markush Bond** () or **Markush Bond with Shadow** () .

**Note:** You can attach more than one fragment using Markush Bonds with Shadow. The second fragment will appear as a shaded Markush bond.


2. To display the attached mass or formula difference values, on the Structure toolbar, click **Markush Bond with Added or Removed Fragment** () or **Markush Bond with Added or Removed Fragment with Shadow** () . In the **Define Markush Mass Difference** dialog box, specify the proper settings and click **OK**.

## Drawing Templates

ChemSketch includes three template tools for drawing structures.

1. **Table of Radicals** ()


This command displays the Table of Radicals containing the most frequently needed radicals for quick structure drawing, e.g. carbon chains, rings, benzene, amino acids, and common protecting groups.

On the References Toolbar, click **Table of Radicals** () . When you point to a radical in the Table of Radicals, it is displayed in the preview area. To choose a radical for drawing, click the radical

button and the Table of Radicals will be closed and a shadow will be attached to the cursor. You can flip the radical shadow by pressing TAB. Click in the empty workspace or on an atom to add the radical to your structure. You can use the radical shadow as many times as you want until you click with the right mouse button to cancel the mode. When a radical is chosen from the Table of Radicals, its corresponding button is automatically added to the References toolbar.

## 2. Instant Template



The **Instant Template** button allows you to create a current pattern from any structure or selected fragment so that you can insert it anywhere in the workspace or attach it to a structure.

With a structure open in the workspace window, select the part of the structure that you want to reproduce. On the Structure toolbar, click **Instant Template** (). Point to the selected part of the structure and click. The shadow of the selected fragment becomes attached to the cursor. You can flip the shadow by pressing TAB. Move it to the desired location and click to paste. You can use the shadow as many times as you want until you click with the right mouse button to exit the mode.

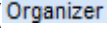
## 3. Template Window

The Template Window allows you to insert predefined, standard structures and graphical objects into your drawing and create your own templates of commonly used structures.

On the General toolbar, click **Open Template Window** ().

In the Template Window, in Structure mode, there are several tabs on the left side of the dialog box that contain standard templates. Click on a tab to view the templates in that group. To navigate through the pages of templates, use the ( ) buttons. To use one of the templates, simply click on the template and it appears as a shadow attached to the cursor. Click to paste the structure on the workspace. Click the right mouse button to remove the shadow from the cursor.

To create a new template, draw the structures that you want included in the template in the workspace window and save them as a ChemSketch file. From the **Templates** menu, choose **Save User Template**. In the **Save User Template** dialog box, specify the name of the template and the location of the file. Click **OK**. Once your document is saved as a user template, the name you specified is automatically added to the list of templates in the Templates window.

In the Template Window, the **Template Organizer** () allows you to manage the standard (built-in) and custom (user-defined) templates.

**Note:** For more information on the Template Organizer, refer to the online help.

## 4. Dictionary

The Dictionary contains ca. 169,000 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.

**Note:** It is possible to add your company's registered compounds to the dictionary for internal use. Please contact us for more information.

## Conclusion

This guide is intended to help you get started. More detailed information is available in the *ACD/ChemSketch Tutorial*, and in the software help files. The User's Guide is available from the **Windows Start menu > All Programs > ACDLABS 2017 > GUIDES**. Online help is accessible from the ChemSketch window, **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.

