



ACD/Web Search Add-On for ChemSketch

Version for Microsoft Windows

User's Guide

***Searching for the Chemical Data
on the Web***

Advanced Chemistry Development, Inc.

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Before You Begin

Thank you for purchasing ACD/Labs software. We have endeavored to produce innovative software that aids chemical research scientists worldwide with spectroscopic validation of structures, elucidation of unknown substances, chromatographic separation, medicinal chemistry, preformulation of novel drug agents, systematic nomenclature generation, and chemical patenting and publication.

About This Guide

This guide provides a description of installing the ACD/Web Search Add-On for ChemSketch and using it to search through the eMolecules, PubChem, and ChemSpider online chemical databases.

The screen shots shown throughout this guide have been taken with a relatively small window size.

This guide is provided in electronic form, readable with Adobe software. If you cannot locate an index topic you need, please do a text string search for the relevant word or phrase, or related words.


Terms

The <ACD> directory is a directory on the hard drive where the ACD/Labs software applications are installed.

The <**ACDLABS**> folder is a folder accessible via the Windows **All Programs** menu where the ACD/Labs software shortcuts are registered.

Mouse Conventions

The following specific words are used to describe mouse procedures throughout this document:

- **Point to** means move the mouse pointer  to an item.
- **Click** or left-click means point to an item, and quickly press and release the left mouse button.
- **Right-click** means point to an item, and quickly press and release the right mouse button.
- **Double-click** means point to an item, and quickly press and release the left mouse button twice.

- **Drag** means point to an item, press and hold down the left mouse button while you move the item.
- **Select** means highlight or make an interface element active by either clicking it or dragging over it (other actions are possible if specified in documentation). If used in "select the check box", it means that the check box should be marked with a tick (as opposed to "clear the check box" when the check box should be cleared, without a mark).

For More Information...

To see the latest in ACD/Labs software and services, please visit our Web site at

<http://www.acdlabs.com>

Our Web site is being accessed at the rate of tens of thousands of "hits" per day. There's a reason for this: much is offered through our Web site. There are TechSmith Camtasia-based movies which show the operation of many of our software packages (especially ACD/ChemSketch). The movies can be run from the ACD/Labs software folder, <ACD>\MOVIES.

We are constantly updating the information on our Web site. The Web site will tell you at which scientific conferences you can visit the ACD/Labs booth. You can browse the Frequently Asked Questions page or drop in and "chat" on our newsgroup, which can also be reached via our Web site.

If you would like to stay informed of the latest developments in chemical software at ACD/Labs, please be sure to sign up for e-mail broadcasts at our Web page:

<http://www.acdlabs.com/newsletters>

How to Contact Us

We are accessible through our Web site, phone, fax, and regular mail, but by far the most popular way to contact us is via electronic mail. Questions on pricing, sales, availability, and general issues should be directed to:

info@acdlabs.com

Technical and scientific support issues should be addressed by visiting:

<http://www.acdlabs.com/support>

Please tell us the name of the software purchaser; the product name, version number, build number, and license ID of the product you are contacting us about (from the **Help** menu, choose **About** to find this information); as well as a description of the problem you are having. If applicable, please tell us the name of the distributor from whom you purchased the software.

Online Updates

Updates of our Desktop and Enterprise products are made throughout the year. These intermediate releases (bringing the actual version number of a program, for example, from *N.00* to *N.01*) often contain new functionality along with additional bug fixes and support for new file formats. To check if there is a new update available and to have this sent to you, please contact your local agent or our Technical Support Department. Before calling, we recommend that you have ready the name of the software purchaser, the product name, version number, build number, and license ID of the product you are contacting us about.

All Desktop ACD/Labs software contains the capability to have software updates delivered online. You will need the registration numbers of the software and an Internet connection from the same computer on which the software is installed. For more information, refer to the *ACD/Updater User's Guide* located in the ACD/Labs documentation folder, <ACD>\DOCS\UP_CLNT.PDF.

1. Introduction

There is a growing prevalence of Web-based portals for searching chemical structures and associated information. In particular the PubChem project initiated by the National Library of Medicine (<http://pubchem.ncbi.nlm.nih.gov/>) has revolutionized online access to millions of chemical structures and an abundance of associated information. PubChem provides information on the biological activities of small molecules and is a component of NIH's [Molecular Libraries Roadmap Initiative](#). PubChem includes substance information, compound structures, and bioactivity data in three primary databases, [PCSubstance](#), [PCCompound](#), and [PCBioAssay](#), respectively.

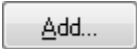

The eMolecules (<http://www.emolecules.com/>)—originally known as Chmoogle—was announced as the leading open-access chemistry search engine. eMolecules' mission is to discover, curate and index all of the public chemical information in the world, and make it available to the public for free.

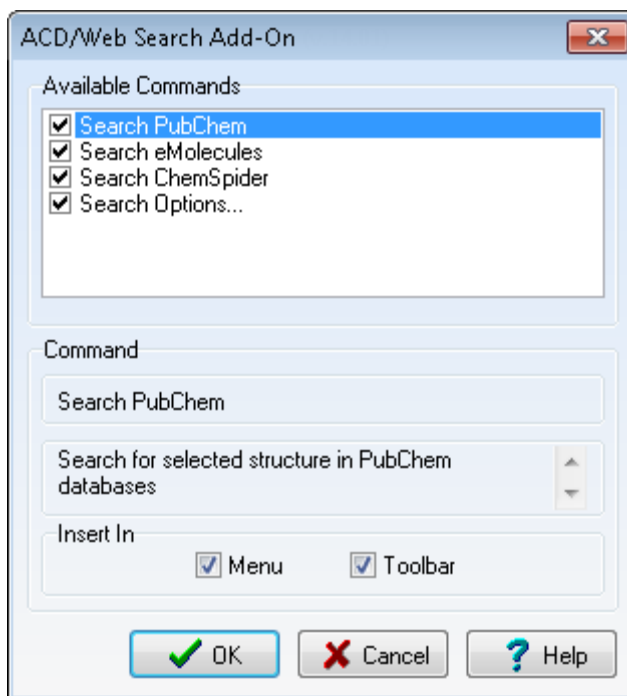
Another one chemistry search engine is ChemSpider which offers you chemical structure searches available online and delivered with the flexibility and usability necessary to encourage repeat usage.

ACD/ChemSketch freeware has now been downloaded by over half a million chemists worldwide and is fast becoming the standard chemical structure-drawing package with the largest install base in the marketplace. In order to deliver further value and support to our users we have provided ChemSketch with a tool that allows both structure and substructure searching of the eMolecules, PubChem, and ChemSpider online repositories. This document describes how to integrate the ACD/Web Search Add-On into the ACD/ChemSketch application installed at your desktop.

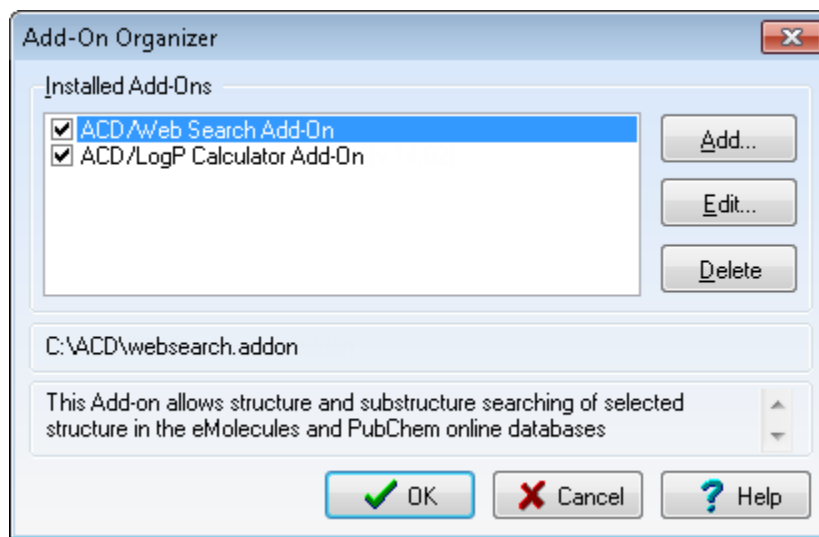
2. Working with ACD/Web Search Add-On

2.1 Installing the Add-On




1. In ACD/ChemSketch (Freeware or Commercial), from the **Options** menu, choose **Add-On Organizer** to display the **Add-On Organizer** dialog box.
2. In the dialog box, click .
3. In the **Open** dialog box that appears, specify the location of the <ACD>\WEBSEARCH.ADDON file, and click .
4. The **ACD/Web Search Add-On** dialog box that follows contains a list of available commands within the add-on and options for placing the commands on the **Add-Ons** menu and/or the General toolbar of the ChemSketch window. Ensure that all of the check boxes are selected as shown below:

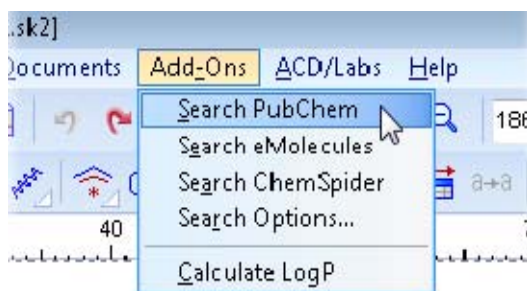


5. Click **OK**, and the new **ACD/Web Search Add-on** entry will appear in the **Installed Add-Ons** list of the **Add-On Organizer** dialog box:



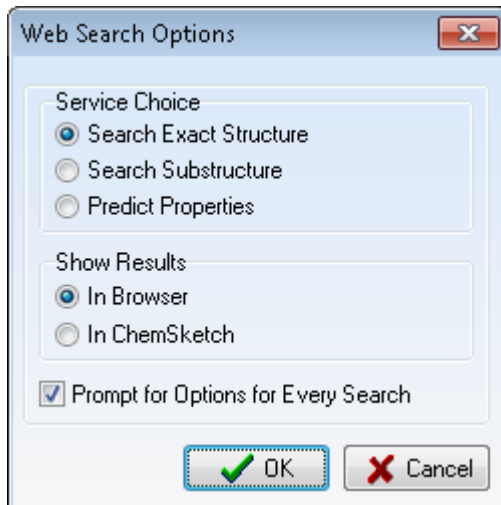
6. Click **OK** to apply the changes and close the dialog box.

As you can see the , , and  buttons now appear on the General toolbar of the ChemSketch window and the group of respective commands is added on the **Add-Ons** menu:



2.2 Choosing Web Search Options

1. From the **Add-Ons** menu, choose **Search Options** to display the following dialog box:



2. In the **Service Choice** area, select either **Search Exact Structure** if you want to perform a search by the complete molecular structure or **Search Substructure** to perform a substructure search.

Note **Predict Properties** are available only for ChemSpider search.

3. In the **Show Results** area, select either **In Browser** if you want to view the results in your Web browser or **In ChemSketch** to display them in the ChemSketch window.

Note This add-on only works with MS Internet Explorer as the Web browser.

4. Click **OK** to apply settings and close the dialog box. You can change these search options at any time depending on the type of search you want to perform.

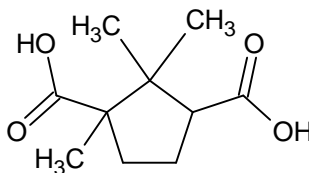
Tip If you select the **Prompt for Options for Every Search** check box, this dialog box will appear every time you start searching through either the eMolecules or PubChem online databases.


2.3 Performing a Web Search on eMolecules

This example will show how to perform a search with the eMolecules service.

Note Performing a search on the PubChem service follows the same procedure (refer to the next section).

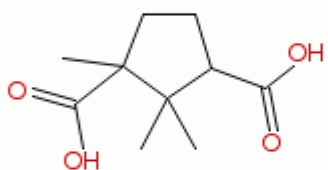
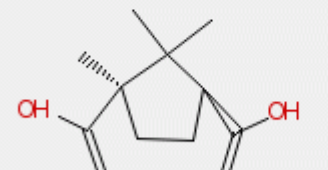
1. Draw or load a structure for *camphoric acid* into the ChemSketch window:



2. On the General toolbar, click  (or choose **Search eMolecules** from the **Add-Ons** menu).

If you chose to show search results in a Web browser, Internet Explorer will load the eMolecules search Web site and display the results of the search after a few moments:

The screenshot shows the eMolecules website interface. At the top, there is a navigation bar with links: Home, Information, My Account, My Lists, Help, and Login. Below this is the eMolecules logo and a "Give us your feedback" link. A "New Search" button is visible. The search results are displayed as "Results 1-4 of 4 (0.6 sec)". A red button "Want to see Prices?" is present. A yellow box contains the text "Click here to Work with this List" and a list of actions: Sort & Filter, Save the list, Change columns/view, and Share, Export, & more.

Structure	MolWt	Supplier	Supplier's ID
 View compound info Edit	200.232	ChemDiv	3232-1238
		Enamine	Z57127432
		InterBioScreen	BB_SC-6478
		Otava	0125160262
		more... (2 total)	
		Vitas M Labs	STL163321
		more... (2 total)	
		TCI America	C0012
		TCI Europe	C0012
TCI Japan	C0012		
 View compound info Edit	200.232	Acros Organics (US)	10820
		Combi-Blocks	OR-1430
		Sigma Aldrich	C409
		Alfa Aesar (US)	B23106
		Bosche Scientific	C1178
		MP Biomedicals	05211802
		Bepharm	B31676
		Santa Cruz Biotechnology	sc-229841
		AK Scientific	68564
		Fluorochem (Non-US Customers)	225471
Ark Pharm	AK-47796		

Otherwise, if you chose to show the results in ACD/ChemSketch, the **Search Results** window will open:

Search Results

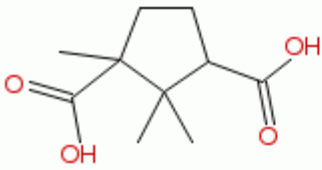
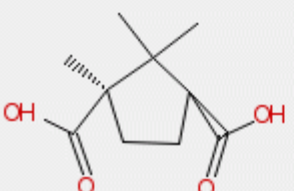
Home | Information | My Account | My Lists | Help | Login

eMolecules [Give us your feedback](#)

New Search **Want to see Prices?**

Results 1-4 of 4 (0.5 sec)

Click here to **Work with this List** • Sort & Filter • Change columns/view
• Save the list • Share, Export, & more

Structure	MolWt	Supplier	Supplier's ID
 View compound info Edit	200.232	ChemDiv	3232-1238
		Enamine	Z57127432
		InterBioScreen	BB_SC-6478
		Otava	0125160262
		more... (2 total)	
		Vitas M Labs	STL163321
		more... (2 total)	
		TCI America	C0012
		TCI Europe	C0012
TCI Japan	C0012		
 View compound info Edit	200.232	Acros Organics (US)	10820
		Combi-Blocks	OR-1430
		Sigma Aldrich	C409
		Alfa Aesar (US)	B23106
		Bosche Scientific	C1178
		MP Biomedicals	05211802
		Bepharma	B31676
		Santa Cruz Biotechnology	sc-229841

<http://www.emolecules.com/cgi-bin/search?q=%43%43%31%28%43%43%43%28%43%28%3D%4F%>

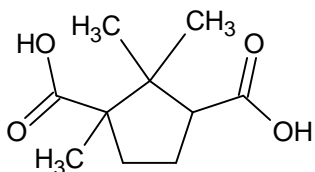
Now you can browse the information in the search results.


2.4 Performing a Web Search on PubChem

This example will show how to perform a search with the PubChem service.

Note Performing a search on the eMolecules service follows the same procedure (see above).

1. Draw or load a structure for *camphoric acid* into the ChemSketch window:



2. On the General toolbar, click  (or choose **Search PubChem** from the **Add-Ons** menu).

If you chose to show search results in a Web browser, Internet Explorer will load the PubChem search Web site and display the results of the search after a few moments:

The screenshot shows the PubChem website interface. The browser window displays the URL [http://pubchem.ncbi.nlm.nih.gov/compound/Camphoric acid](http://pubchem.ncbi.nlm.nih.gov/compound/Camphoric%20acid). The page title is "Camphoric acid - Compound Summary (CID 21491)". The page content includes the following information:

- Also known as:** (+)-Camphoric acid, d-Camphoric acid, Dextro-camphoric acid, 1,2,2-Tricarboxylic acid, 124-83-4
- Molecular Formula:** C₁₀H₁₆O₄ **Molecular Weight:** 200.23164 **InChIKey:** LSPHULW...

On the left side, there is a "Table of Contents" with links to various sections: Identification, Related Records, Literature, Patents, Biological Test Results, Classification, and Chemical and Physical Properties. Below the table of contents is a button labeled "Expand all sub-sections". On the right side, there are two tabs: "2D Structure" and "3D Conformer". The "2D Structure" tab is selected, and it displays the chemical structure of camphoric acid.

If you chose to show the results in ACD/ChemSketch, then the **Search Results** window will open:

Search Results

NCBI

PubChem
Compound

PubChem Compound Limits Advanced search

SHARE

Camphoric acid - Compound Summary (CID 21491)

Also known as: (+)-Camphoric acid, d-Camphoric acid, Dextro-camphoric acid, 1,2,2-Trimdicarboxylic acid, 124-83-4

Molecular Formula: $C_{10}H_{16}O_4$ Molecular Weight: 200.23164 InChIKey: LSPHULWDV

Table of Contents Show subcontent titles

- Identification
- Related Records
- Literature
- Patents
- Biological Test Results
- Classification
- Chemical and Physical Properties

Expand all sub-sections

2D Structure 3D Conformer

Chemical structure diagram of Camphoric acid (CID 21491) is shown, featuring a bicyclic system with two carboxylic acid groups.

<http://pubchem.ncbi.nlm.nih.gov/search/search.cgi>

Now you can browse the information in the search results.