

ACD/Web Search Add-On for ChemSketch

Version 11.0 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.

The colors and other properties of the window elements described throughout this guide correspond with the default Windows Display Properties.

This guide is provided in electronic form, readable with Adobe Acrobat 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.

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. As of Fall 2006, we offer free ChemSketch 10.0, an ACD/LogP Freeware Add-on for ChemSketch, a free ISIS 3D Add-in, free ChemDraw extensions, and a free 2-week demo key for "Interactive Laboratory" sessions where you can run test calculations using Java applets without purchasing software. There are TechSmith Camtasia-based movies which show the operation of many of our software packages (especially ACD/ChemSketch) available for download.

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 page.

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 site page:

<http://www.acdlabs.com/feedback/mailing.html>

If you would like to participate in the ACD/Labs forums, please access:

<http://forum.acdlabs.com>

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://support.acdlabs.com>

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

All PC-based 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. The updates are small fixes, for example, bringing the actual version number of a program from 11.00 to 11.01. For more information on this, refer to the *ACD/Updater User's Guide* located in the ACD/Labs documentation folder, \\DOCS\\UP_CLNT.PDF, or contact our Technical Support Department.

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.

Recently 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.

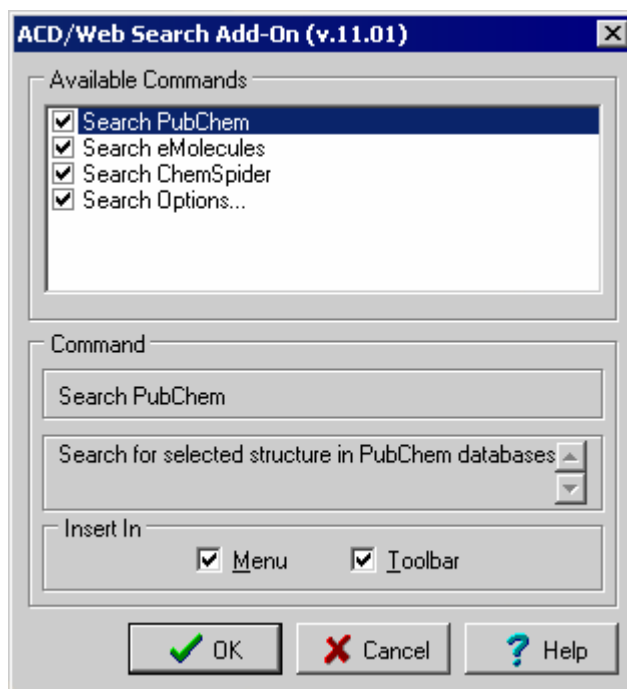
Another one chemistry search engine is ChemSpider which offers you chemical structure searches available online and delivered with the flexibility and usability necessary to encourage repeat usage.

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.

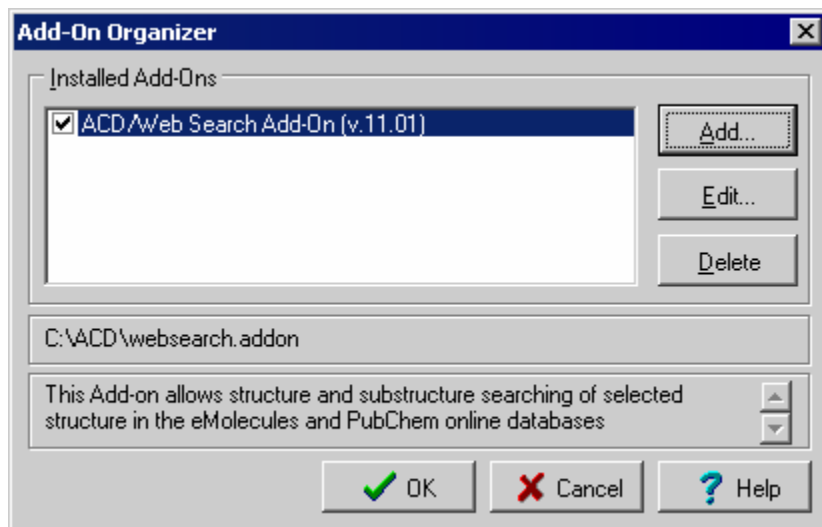
2. Working with ACD/Web Search Add-On




2.1 Installing the Add-On

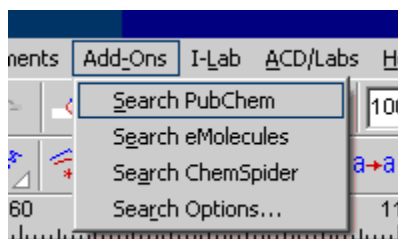
1. In ACD/ChemSketch (Freeware or Commercial), from the **Options** menu, choose **Add-On Organizer** to display the **Add-On Organizer** dialog box.
2. In the dialog box, click **Add**.
3. In the **Open** dialog box that appears, specify the location of the WEBSEARCH.ADDON file, and click **Open**.
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. Make sure that all check boxes are selected as shown below:



5. Click **OK** and make sure that the **ACD/Web Search Add-on** item appears in the **Installed Add-Ons** list of the **Add-On Organizer** dialog box:

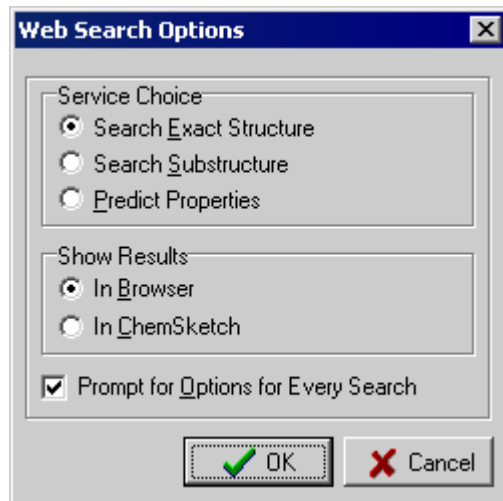


Click **OK**. The **Search eMolecules** , **Search PubChem** , and **Search ChemSpider**  buttons will appear on the General toolbar of the ChemSketch window and the corresponding commands will be added on the **Add-Ons** menu:



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.

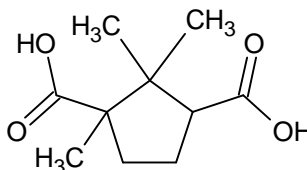
Tip If you select the **Prompt for Options for Every Search** check box, this dialog box will appear every time you start searching through either the eMolecules or PubChem online databases.

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 **Search eMolecules**  (or from the **Add-Ons** menu choose **Search eMolecules**).

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:


eMolecules Chemical Search Results - Microsoft Internet Explorer

File Edit View Favorites Tools Help

Back Forward Stop Home Search Favorites Reload Print W >>

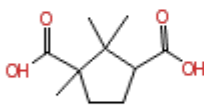
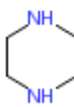
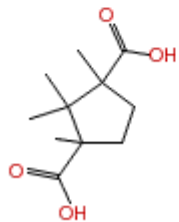
Address <http://www.emolecules.com/cgi-bin/search?q=%43%43%31%28%43%4> Go Links >>

eMolecules® Home

New Search  Draw Structure Text Search

Results for: OC(=O)C1CCC(C)(C(=O)O)C1(C)C

Searched 6.3M structs from 15.4M sources Results 1-7 of 7 (0.9 sec)


NH3		MW: 200.23 ACDlogP: 1.47	PubChem , PubChem Compounds 688016 , CAS: 5985-93-3
details	edit		
		MW: 200.23 ACDlogP: 1.47	National Cancer Institute , August 2000 2D File: 37542 86838 , CAS 999-99-9 999-99-9 PubChem , PubChem Compounds 123663 93874
details	edit		

Internet


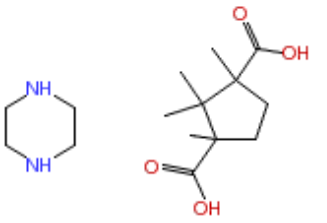

Otherwise, if you chose to show the results in ACD/ChemSketch, the **Search Results** window will open:

Search Results

eMolecules® [Home](#)

New Search  Draw Structure Text Search

Results for: OC(=O)C1CCC(C)(C(=O)O)C1(C)C
 Searched 6.3M structs from 15.4M sources Results 1-7 of 7 (0.3 sec)

 details edit	MW: 200.23 ACDlogP: 1.47 PubChem , PubChem Compounds: 688016 , CAS: 5985-93-3
 details edit	MW: 200.23 ACDlogP: 1.47 National Cancer Institute , August 2000 2D File: 37542 86838 , CAS 999-99-9 999-99-9 PubChem , PubChem Compounds: 123663 93874
 details edit	MW: 200.23 NIST Chemistry WebBook , NIST

<http://www.emolecules.com/cgi-bin/search?q=%43%43%31%28%43%43%43%28%43%28%4F%29%3D%4F%>

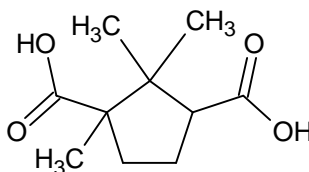
Now you can browse the information in the search results.

2.4 Performing a Web Search on PubChem

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

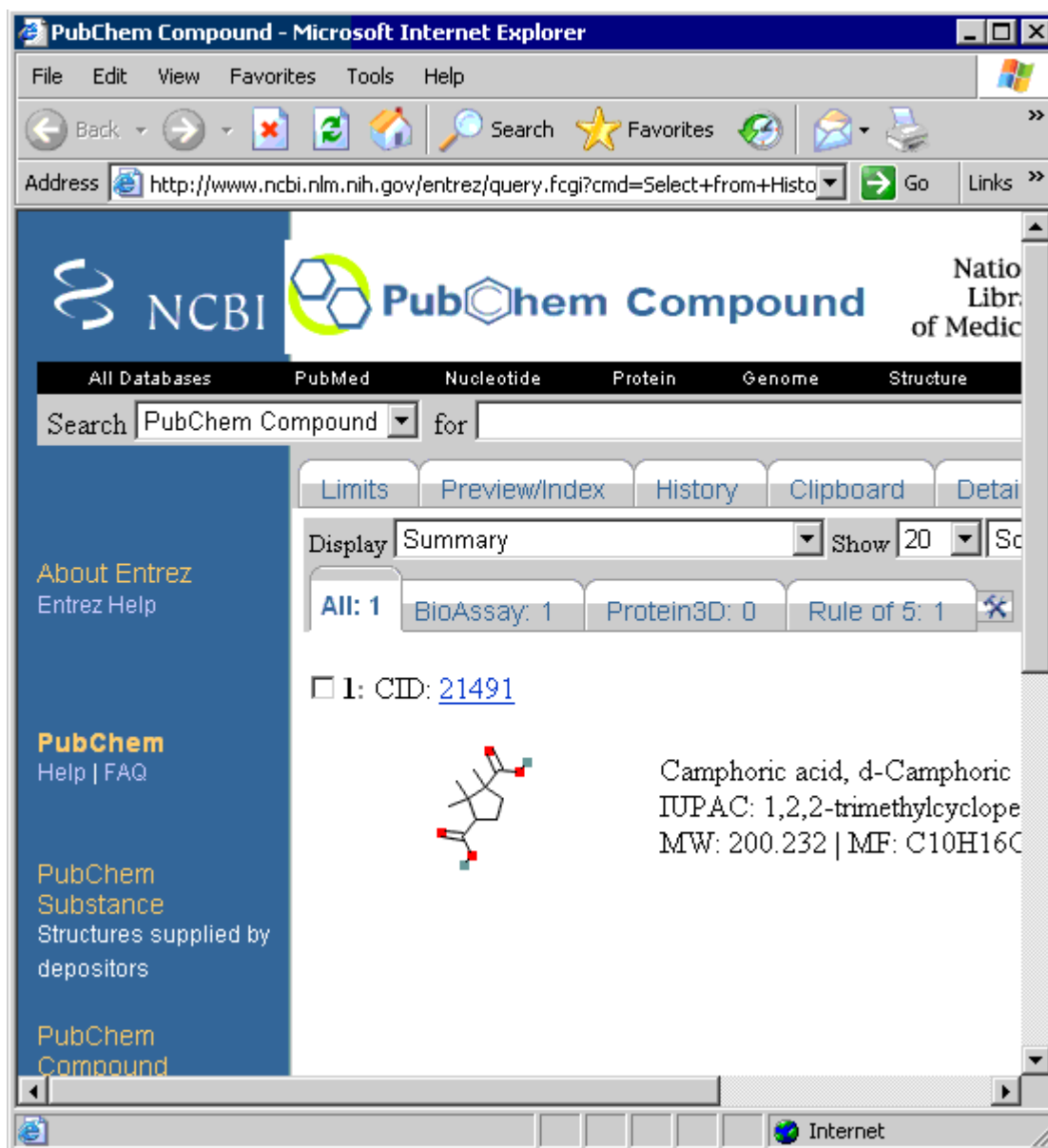
Note Performing a search on the eMolecules service follows the same procedure (see above).

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



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

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:



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

The screenshot shows the 'Search Results' window from the NCBI PubChem Compound database. The window title is 'Search Results'. The header includes the NCBI logo and 'PubChem Compound' with the National Library of Medicine logo. A navigation bar contains links: 'All Databases', 'PubMed', 'Nucleotide', 'Protein', 'Genome', 'Structure', and 'PubChem'. A search bar shows 'PubChem Compound' selected. Below the search bar are tabs: 'Limits', 'Preview/Index', 'History', 'Clipboard', and 'Details'. The 'Display' dropdown is set to 'Summary', and 'Show' is set to '20'. A summary bar shows 'All: 1', 'BioAssay: 1', 'Protein3D: 0', and 'Rule of 5: 1'. The main content area displays the first result: '1: CID: [21491](#)'. To the right of the result is a chemical structure of Camphoric acid, d-Camphoric acid, with its IUPAC name '1,2,2-trimethylcyclopentane-1,2-dicarboxylic acid' and molecular weight 'MW: 200.232 | MF: C10H16O4'. The left sidebar contains links for 'About Entrez', 'Entrez Help', 'PubChem', 'Help | FAQ', 'PubChem Substance', 'Structures supplied by depositors', 'PubChem Compound', 'Unique structures with computed properties', and 'PubChem BioAssay', 'Bioactivity assay results supplied by'. The status bar at the bottom shows the URL 'http://pubchem.ncbi.nlm.nih.gov/search/PreQ5rv.cgi'.

Now you can browse the information in the search results.