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.

Table of Contents

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.

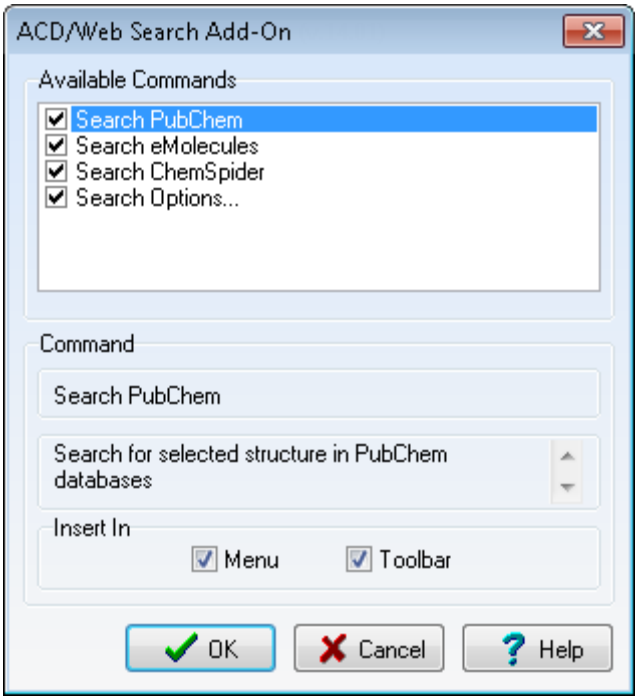
Another one chemistry search engine is ChemSpider which offers you chemical structure searches available online and delivered with the flexibility and usability necessary to encourage repeat usage.

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.

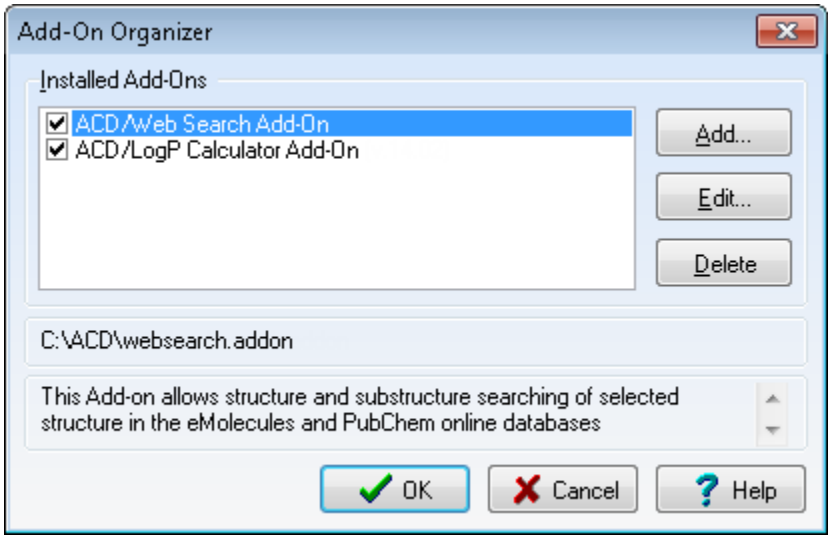
2. Working with ACD/Web Search Add-On

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 Add... .
3. In the **Open** dialog box that appears, specify the location of the <*ACD*>\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. Ensure that all of the check boxes are selected as shown below:

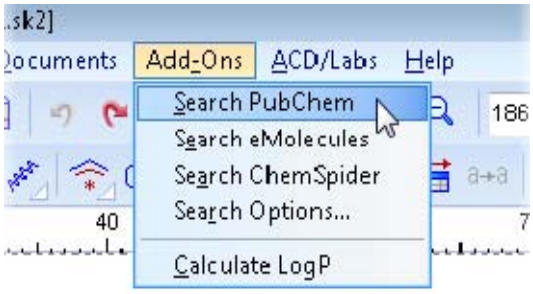


5. Click **OK**, and the new ***ACD/Web Search Add-on*** entry will appear in the **Installed Add-Ons** list of the **Add-On Organizer** dialog box:



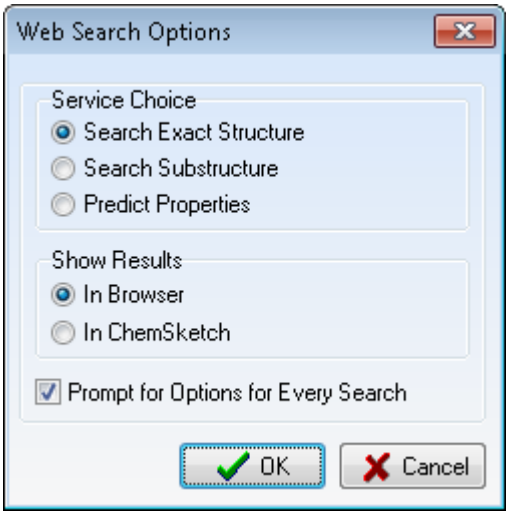
6. Click **OK** to apply the changes and close the dialog box.

As you can see the PubChem, eMolecules, and ChemSpider 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.

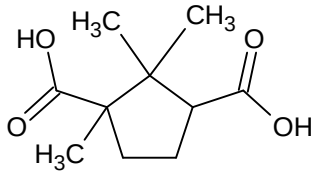
> **Tip** If you select the **Prompt for Options for Every Search** check box, this dialog box will appear every time you start searching through either the eMolecules or PubChem online databases.

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).

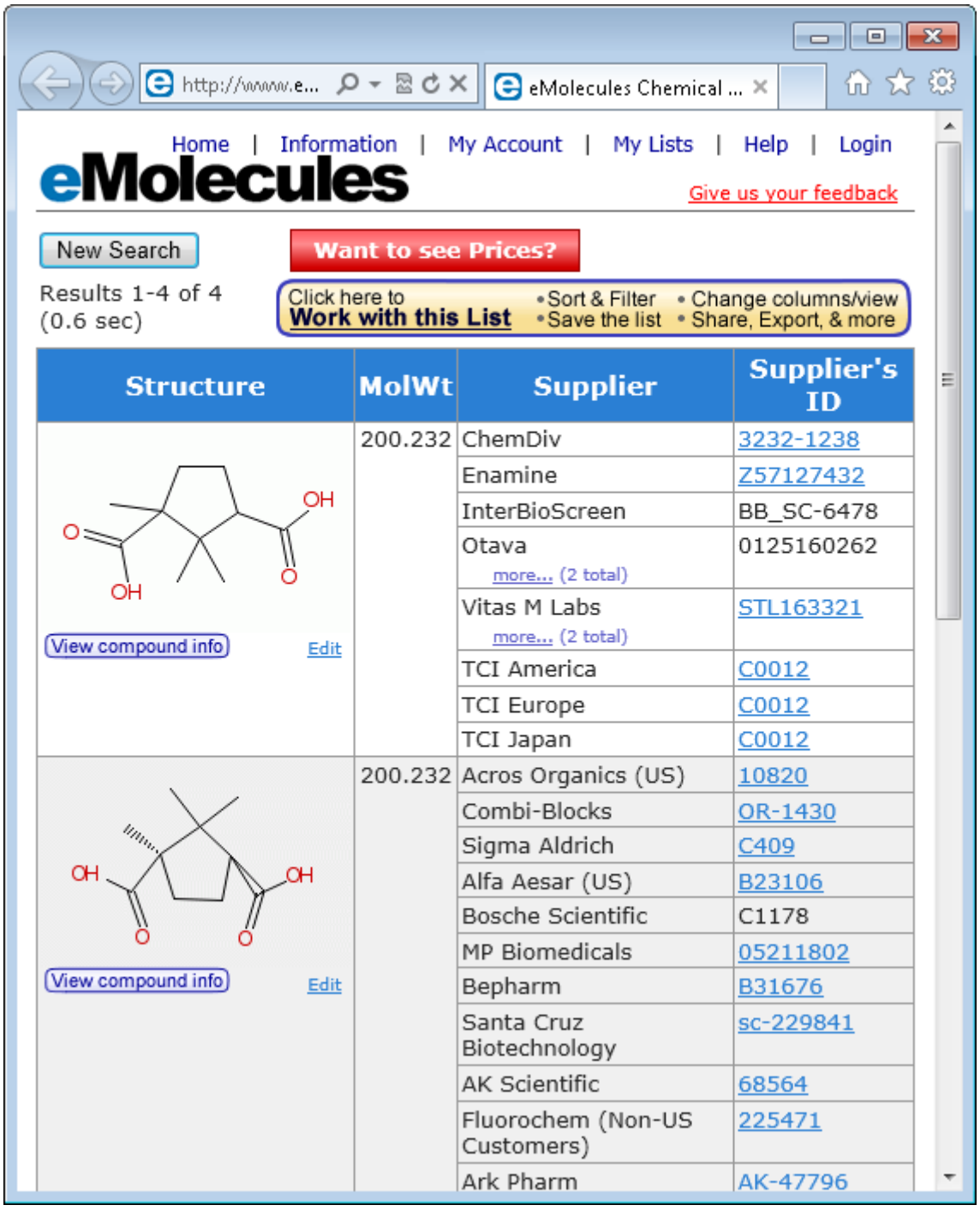
1. Draw or load a structure for *camphoric acid* into the ChemSketch window:



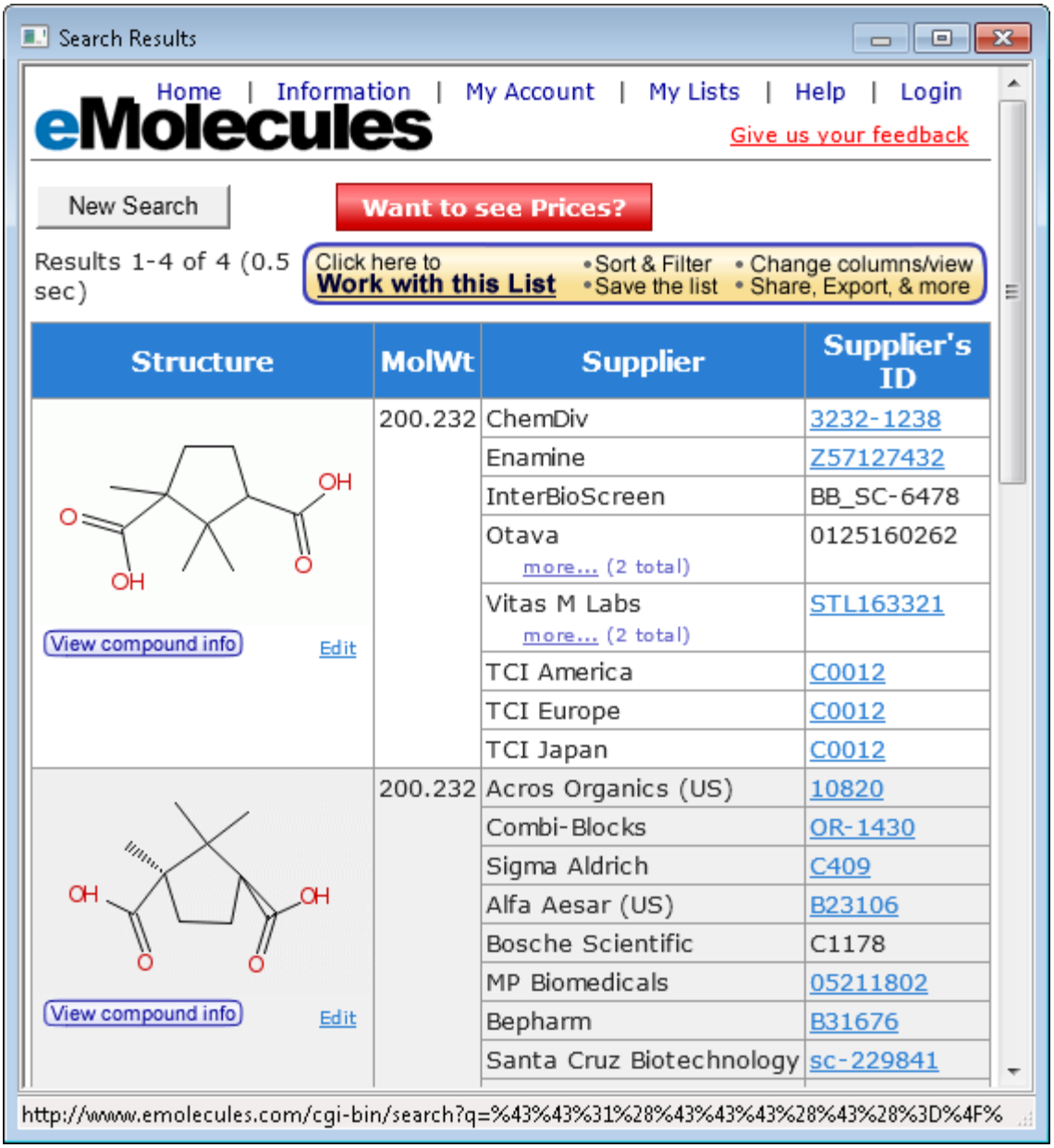
2. On the General toolbar, click 

(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:



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



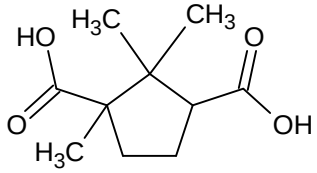
Now you can browse the information in the search results.

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).

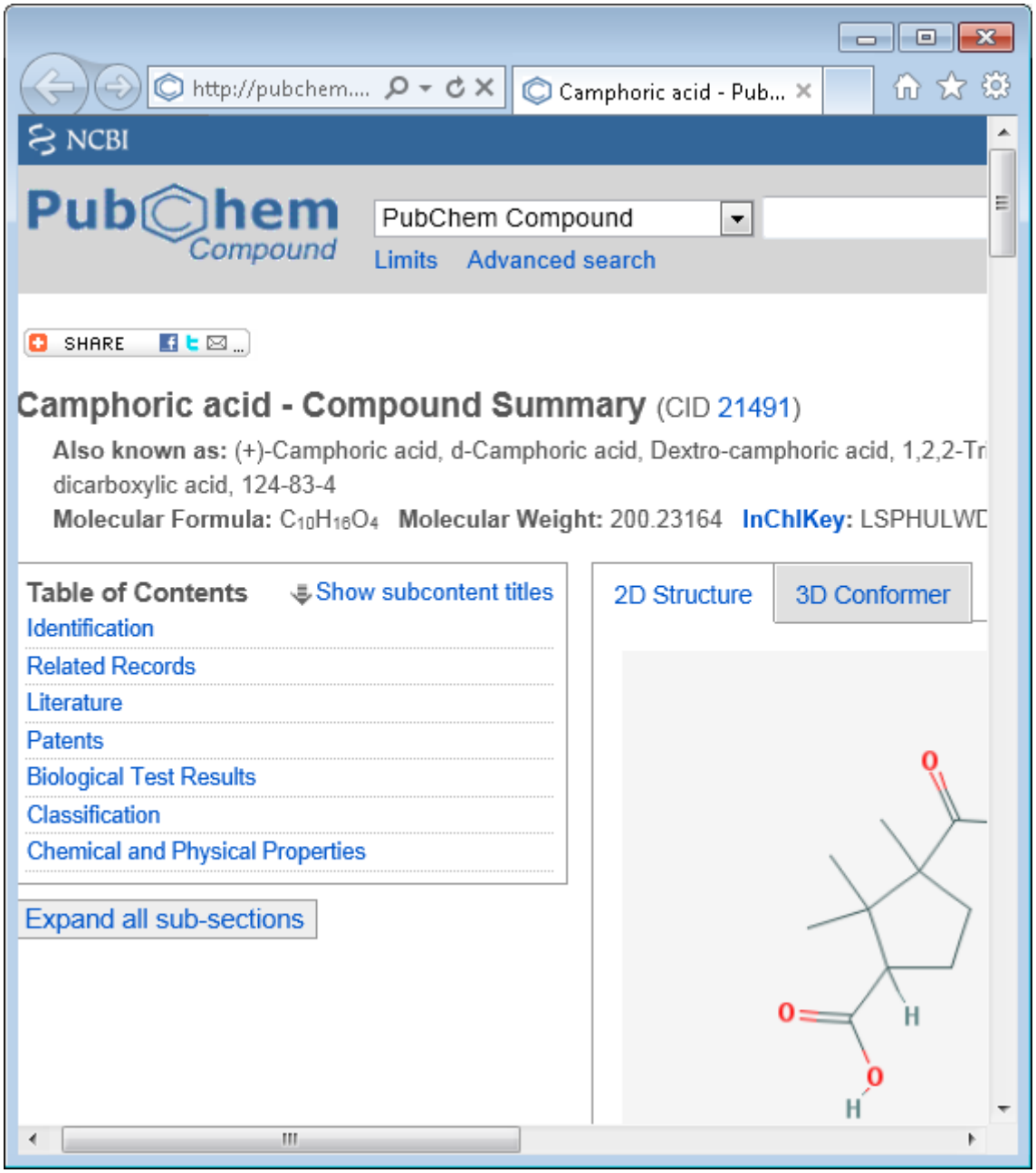
1. Draw or load a structure for c*amphoric acid* into the ChemSketch window:



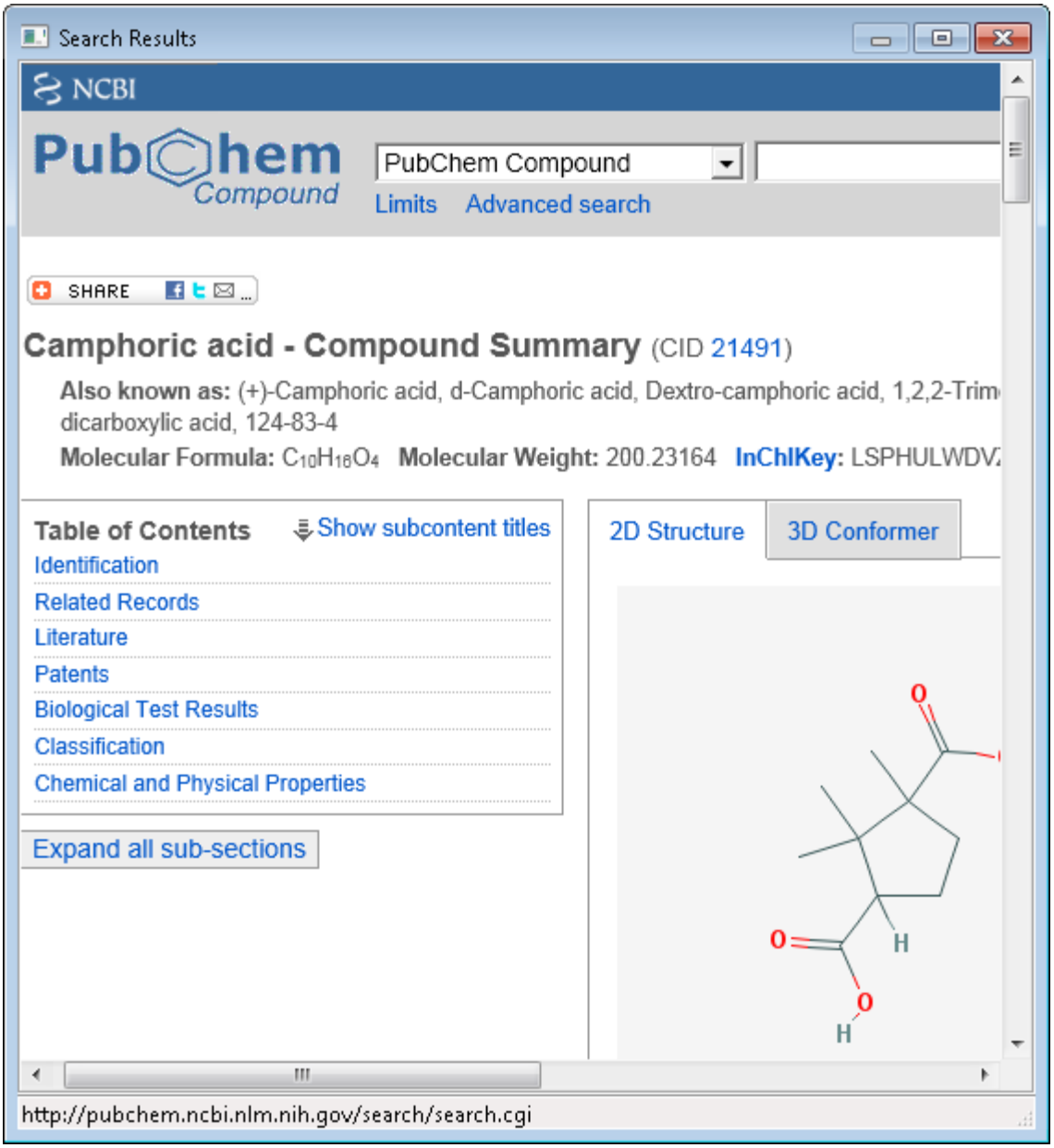
2. On the General toolbar, click 

(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:



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



Now you can browse the information in the search results.