

Integrating ACD/ChemSketch to ChemSpider for Online Property Prediction and Searching

BETA RELEASE

Online Property Prediction and Structure Searching

Introduction

ChemSpider is a chemistry search engine. It has been built with the intention of aggregating and indexing chemical structures and their associated information into a single searchable repository and making it available to everybody, at no charge. ChemSpider is a value-added offering since many properties have been added to each of the chemical structures within the database – structure identifiers such as SMILES, InChI, IUPAC and Index Names as well as many physicochemical properties. ChemSpider also offers online access to a series of prediction engines to allow users to predict these properties, in real time, for their own molecules of interest. This technical note explains how the desktop structure drawing software, ACD/ChemSketch, can be used to access both the property predictions as well as the ability to perform searches of the database.

ACD/ChemSketch Freeware Overview

ACD/ChemSketch is likely the most popular freeware chemical structure drawing package in the world today with over 750,000 downloads around the world and hundreds of site licenses across academia. The freeware software can be downloaded from <http://www.acdlabs.com/download/> and manuals are available in various languages at <http://www.acdlabs.com/download/#Guide> to serve various parts of the chemical community . The websearch addon can be downloaded from <http://www.acdlabs.com/download/#free>.

Setting up the WebSearch Addon

Installing the websearch addon is very simple. Simply backup the websearch addon you are presently using by renaming to websearch.old and copy the new websearch addon into the ACD/Labs root directory. Start ChemSketch and the new websearch addon is enabled. For further details please review the technical note regarding websearch addon installation at the ACD/Labs website http://www.acdlabs.com/download/technotes/80/draw_db/websearch.pdf. Following installation at the top of the screen the ChemSpider button illustrated below will be shown.



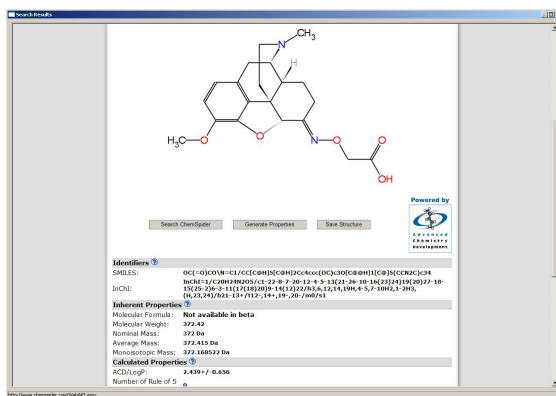


Technical Note

In order to perform a search of the ChemSpider database or predict properties from ChemSketch simply sketch the chemical structure or substructure of interest and click on the ChemSpider button. The dialog box shown below will appear and the service of choice may be selected: either search the exact structure against the database, search for the drawn substructure or predict properties for the drawn structure using the ChemSpider Properties Service.



The results can be shown in either a browser window such as Firefox or Internet Explorer or in a window which pops up over ChemSketch as shown below.



From this window the other operation of interest may be to search the structure in ChemSpider.

Conclusion

ACD/ChemSketch has been integrated into ChemSpider to allow desktop access to searching the database via structure and substructure as well as generation of predicted properties. This development exposes initial efforts to integrate popular drawing packages to the ChemSpider services.