

Adding ChemSpider Searching into your Own Website

Introduction

The ChemSpider chemistry search engine was 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 searches can be accessed via the ChemSpider webpage, via the PC-based desktop drawing package ACD/ChemSketch, via a toolbar add-in for both Internet Explorer and Firefox and now, via your own website. This technical note describes how to perform text-based searches for chemical structures using inputs of systematic names, trade names and synonyms, registry numbers, InChI codes and SMILES strings by embedding the search directly into your webpage

Text-Based Searching

The ChemSpider search page offers two modes of searching, the default search shown below as well as an advanced search (allow searching by structure/substructure and molecular properties).



The simple search screen allows searching based on Systematic Name, Synonym, Trade Name, SMILES string or InChI string. The search works by first searching on the synonym. If nothing is found then it converts the query to an InChI string if possible (using ACD/Labs Name to Structure conversion software, this also converts SMILES to InChI). If nothing is found using the InChI as the basis of the search then a search is performed using the originally input text to search as a substring of a synonym.

This text-based search has been enabled from within a browser window by providing add-ins to incorporate into the browser window following the OpenSearch standard.



Adding ChemSpider Text Searching into your Webpage

Below we list an example of the HTML code necessary to enable a ChemSpider search from your website. We assume that you will understand enough about HTML programming to embed this information into your website:

```
<html>
<head>
  <title>Search ChemSpider example</title>
</head>
<body>
<table>
<tr>
<td align="right" valign="middle">
  Form based search:
</td>
<td>
<form action="http://www.chemspider.com/Search.aspx" method="GET">
  <input name="q" type="text" value="viagra" />
  <input type="submit" value="Search on ChemSpider!" />
</form>
</td>
</tr>
<tr>
<td align="right">
  Link based search:
</td>
<td>
<a href="http://www.chemspider.com/Search.aspx?q=viagra">Viagra</a>
</td>
</tr>
</table>
</body>
</html>
```



Technical Note

Test the searching using the following example text strings..copy and paste the string following the colon

- 1) Systematic name: search 6-(bromoethynyl)-2H-pyran-2-one
- 2) Trade Name: search xanax
- 3) Registry Number: search 80356-14-5
- 4) SMILES string: search Clc3cc2\C(=N/Cc1nnc(n1c2cc3)C)c4cccc4
- 5) InChI string: search

InChI=1/C5H11NO2/c1-6(2,3)4-5(7)8/h4H2,1-3H3/p+1/fC5H12NO2/h7H/q+1

Conclusion

The ChemSpider text-based searches have been made available as add-ins for both Internet Explorer and Firefox web browsers and can now be embedded directly into your webpage. This technical note has provided an overview of how to code this capability into your webpage to facilitate ease-of-use. As usual, if there are issues with this capability please provide us feedback at bugs@chemspider.com.