

Sharing Product Physical Characteristics over the Internet

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Abstract: This paper presents a new method that allows organic chemists to share information about new and existing chemicals over the Internet. Everybody is free to submit and retrieve information. This database is readily accessible from the Internet at <http://ccd.chemexper.com>.

Introduction

The Internet has reached an important place in the everyday life of a chemist¹. A lot of information is available in the form of on-line journals, job banks, conference announcements, etc. New applications such as WebElements²; VchemLab³ or TeleSpec⁴ as well as new standards, specific to chemistry, are emerging⁵ and benefit from the possibilities offered by the Internet. Various databases containing chemicals have appeared. Among them, some are available at no cost, such as ChemFinder⁶, and others require a paid account. However, all those databases share common limitations:

- The scientist that has determined the physical characteristics of a chemical can never provide directly the information to the database. Indeed, his results have first to be published, then indexed, before finally being incorporated into a database.
- The databases require a lot of centralized management. Usually the data is selected from reviews of the literature or from other databases.

In this article we would like to present a new way for organic chemists to share chemical information over the Internet. Everybody can contribute to this freely accessible database that requires limited management.

General principle

We have developed a web server (<http://ccd.chemexper.com>) to which anybody can contribute using our application that can be downloaded from our server. This database is called "ChemExper Chemical Directory" and contains chemical compounds as well as their physical characteristics.

The originality of this database lies in the way it keeps track of the information. Indeed, it remembers who is the submitter of all the information present in the database. After making a query (Figure 1, A) and selecting a product (Figure 1, B), you will see a list of the standard characteristics of the compound (Figure 1, C). This data corresponds to the first person that has submitted a value for a particular analysis. However, for each information a link is still available and will give you access to all the results present for this specific analysis as well as data about who has submitted it (Figure 1, D) (name, e-mail address, etc.).

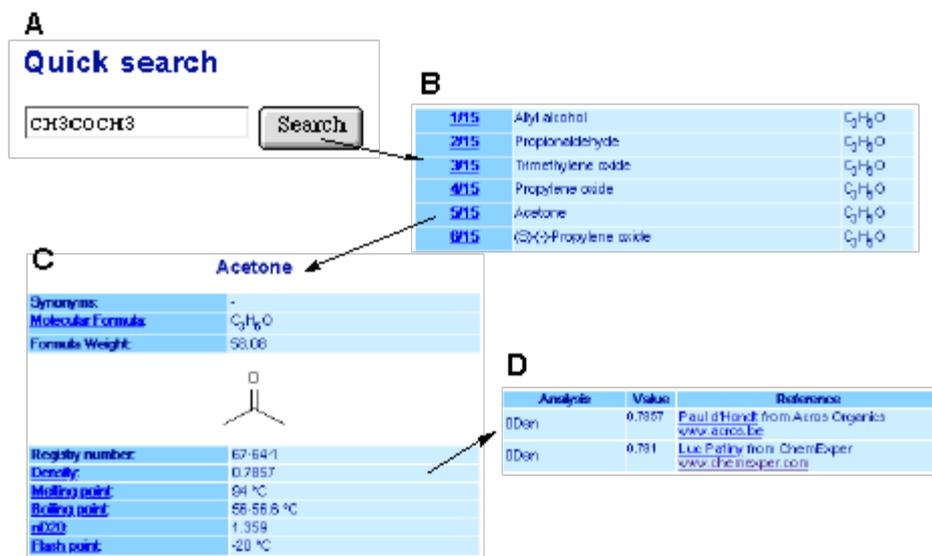


Figure 1

Knowing and showing the source of all the information present in the database present many advantages. Amongst them we may cite:

- the possibility for the person who submitted the information to modify it later.
- the limitation in the number of false information. We expect that people will take more care about the accuracy of information they submit when this data is related to their name.
- for the person looking for information it is much more interesting to see all the values that were submitted, rather than only one value that may be correct or false. This will give a much better idea of possible inaccuracies in the database.

At the user level, this project may be divided in two phases : the submission process and the retrieval process.

Submitting data

Data is submitted to the server using an application called "Expereact WEB". This program runs on PC or Macintosh platforms. It allows the maintenance of local database in each laboratory containing the products that have been characterized. Most of the information about new or existing chemicals can be entered in this program, such as the boiling point, melting point, NMR, IR, etc. (Figure 2).

<>After registering the program, the information may be submitted to our server and it will be immediately accessible to the world. Even after submission, it is still possible to change the data or to add new results. In order to reach this goal, the local database has to be modified and the data resubmitted to the server.

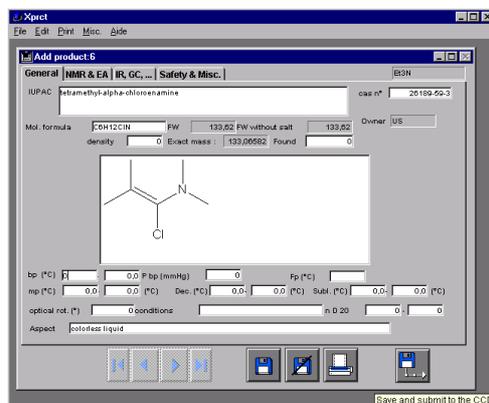


Figure 2

The process of submitting information is particularly easy and only requires to press the "submit to server" button. The program will then send to the server an E-mail containing the characteristics of the selected products. The use of the simple mail transfer protocol (SMTP) to submit information was chosen in order to avoid the need to invent a new protocol and also to avoid potential problems with firewalls.

Retrieving data

Searching in the database can be done using any browser that allows frames. The address of the database is <http://ccd.chemexper.com>. There are several ways to search in the database over the Internet :

Quick searching

The first way to search in the database is the quick search. Molecular formula, a registry number or a product name may be entered for this kind of query. The program will automatically try to find the right field for the search and give back the list of the selected products. This is the fastest and easiest way to find a chemical.

Physical characteristics

The second way to search is a mixed search. This option gives access to a more complex form that allows multiple field searches. For example, it will be possible to mix physical characteristics (boiling point, melting point, etc.) with substructure (SMILES⁷), names or molecular formula.

For the most complex searches it is even possible to use the power search tool that allows the combination of physical and chemical characteristics in a complex Boolean expression including multiple parentheses e.g.: $mp=70\pm 10$ and $(bp=150\pm 5$ or $bp=180\pm 5)$ and $fw < 400$. Those queries may also be performed on NMR chemical shifts or IR maxima.

Substructure searching

Finally the last way to search is the substructure search. The substructure engine is based on a very simple but efficient Java applet that we have developed. It allows a user to directly search in the database without having to download and install a plug-in. The program will automatically check if such an element exists and care should be taken with upper and lower case. The search engine automatically calculates the aromaticity.

Conclusions

In this paper we present the first project that allows chemists to share information over the Internet by sending their data directly to a web server. This tool is very intuitive and easy to use. Moreover, it will allow the chemical scientific community to directly contact other laboratories. Future development will include new possibilities such as a reference database, the possibility to add spectra in the J-CAMP format⁸ and 3D visualization of the molecules.

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References

- 1 Wiggins, G. J. *Chem. Inf. Comput. Sci.* **1998**, *38*, 956-965.
- 2 Developments on the Web-based periodic table database of element properties called WebElements. Mark J. Winter, Abstract number 39 presented at the COMP Division of the 210th American Chemical Society Meeting in Chicago, USA, on 21 August 1995. Rzepa, H. S.; Whitaker, B. J.; Winter, M. J. *J.C.S. Chem. Commun.*, **1994**, 1907-1910.
- 3 Rzepa, S. R.; Tonge, A. P. *J. Chem. Inf. Comput. Sci.* **1998**, *38*, 1048-1053.
- 4 Selzer, P. *Chimia* **1998**, *52*, 678-682.
- 5 Rzepa, H. S.; Murray-Rust, P.; Whitaker, B. J. *J. Chem. Inf. Comput. Sci.* **1998**, *38*, 976-982. Rzepa, H. S. *Chimia* **1998**, *52*, 653-657.
- 6 Brecher, J. S. *Chimia* **1998**, *52*, 658-663.
- 7 Weininger, D. *J. Chem. Inf. Comput. Sci.* **1988**, *28*, 31-36.
- 8 Gasteiger, J.; Hendriks, B. M. P.; Hoever, P.; Jochum, C.; Somberg, H. *Applied Spectroscopy* **1991**, *45*, 4-11. Robert, S.; McDonald, R. S.; Wilks, P. A., Jr. *Applied Spectroscopy* **1988**, *42*, 151-162. Davies, A. N.; Lampen, P. *Applied Spectroscopy* **1993**, *47*, 1093-1099. Lampen, P.; Hillig, H.; Davies, A. N.; Linscheid, M. *Applied Spectroscopy* **1994**, *48*, 1545-1552.