A Free and Fast Chemical Reaction Search

Over the last years, structure-based chemical databases, such as Beilstein, REACCS, and SciFinder, have gained tremendous importance for the synthetic organic chemist. These subscription-based software tools facilitate access to a wealth of valuable information. Due to their structure-centered indexing, both Beilstein and SciFinder are ideal tools for structure queries. An annotation system for organic reactions has only recently been developed at Brandeis University, available as WebReactions (WR).

Hendrickson and Sander have categorized chemical reactions based on bond reorganizations during a given transformation.[1,2] Because of its strict reliance on bond changes, WR is able to carry out reaction queries much faster than Beilstein, REACCS, or SciFinder. When I tested the database, I was indeed impressed with the notably higher speed of data retrieval. In addition to this advantage, WR is a free tool that requires nothing but a Netscape browser. Plugins are not needed, since everything relies on Java and CORBA protocols. However, this freedom comes at a price: Neither Internet Explorer nor the Macintosh OS fully support these standards, forcing the user to stick with the Netscape Navigator/Windows combination.

WR is a recast version of InfoChem's ChemReact database, which contains 401 671 individual reactions abstracted from the primary literature between 1975 and 1991. In comparison to other reaction databases, its limited catalog of years is one of the major drawbacks of WR.

WR is easy to learn and use. The site consists of a well designed and very intuitive interface, similar to what is found in ChemDraw (Figure 1). Five subsections, represented by buttons at the top of the screen, guide the user through the query process. As an example, I attempted to find information on Stille-type couplings. I entered a generic aryl halide and vinyl trimethyltin in the "Define Reactants" module and progressed to the "Define Products" section. Here, the initial drawing reappeared and I simply modified the two reactant structures into a single aryl vinyl species. Upon clicking on "Search Database", nine hits were returned almost instantly along with a submenu to browse the query results. One of WR's key features is the pruning mechanism that narrows down the results to a manageable number of hits (10–20 reactions). To "Fine-tune the Hitlist", users can either adjust the minimum required yield or select any highlighted atom or bond to define additional constraints. Selecting the tin atom, I was very satisfied with the options to modify the query atom: Sn; Sn or Pb; Sn, Pb, Sb, or Bi; B, Si, Ge, Sn, Pb, Sb, or Bi; group 3A–4A; group 1A–5A; any electropositive element; anything. Selecting the "B, Si, Ge, Sn, Pb, Sb, Bi" group, the query results were expanded to 28 hits, to include examples of Suzuki, Stille, and Negishi couplings. Finally, the "Hit Reaction Text" link yielded the literature citation.

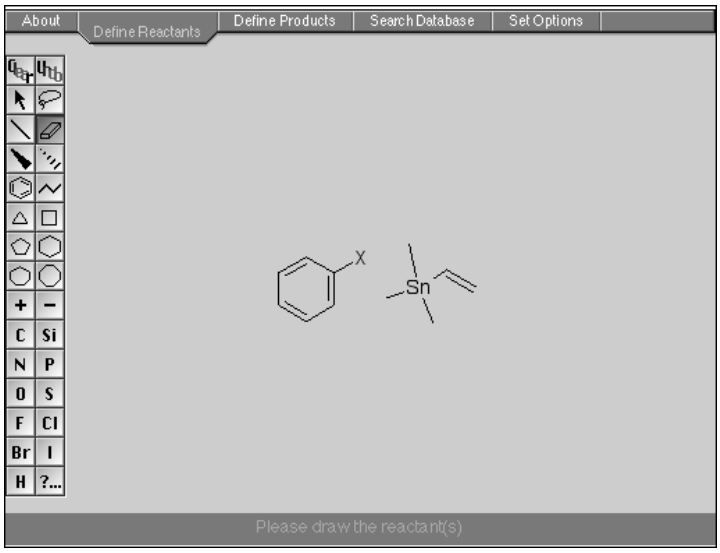

Figure 1. WebReactions' intuitive interface.

Suggest a web site or submit a review:
angewandte@wiley-vch.de

WR is a fast and user-friendly search solution that is available free of charge. It complements existing software tools such as Beilstein or SciFinder, although there is an economic advantage in using WR. However, the browser/OS compatibility problems reduce its appeal, especially in a Macintosh environment. Although WR only covers about 400 000 reactions reported between 1975 and 1991, there is apparently little overlap between many databases, making WR indeed a valuable tool.

Ulrich Iserloh
Memorial Sloan–Kettering Cancer Center, New York, NY

[1] J. B. Hendrickson, T. L. Sander, *J. Chem. Inf. Comp. Sci.* **1995**, *35*, 251; J. B. Hendrickson, T. L. Sander, *Chem. Eur. J.* **1995**, *1*, 449. The COGNOS program for reaction retrieval was eventually renamed Webreactions and launched in 1995 in its present internet-accessible format.
[2] J. B. Hendrickson, L. j. Zhang, *Chem. Inf. Comp. Sci.* **2000**, *40*, 380.

For further information visit:
http://www.webreactions.net/
or contact
hendrickson@brandeis.edu

  1433-7851/02/4115-2851 $ 20.00+.50/0