
COMPUTER SOFTWARE REVIEWS

HYDRO

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HYDRO,¹ version 1.50 for Windows,² is a software package which can estimate aqueous hydrolysis rates of a variety of organic species including esters, carbamates, epoxides, halomethanes, and alkyl halides. It will estimate either acid- or base-catalyzed rates at 25 °C although not neutral (uncatalyzed) rates. It does not deal with temperature dependence of the rates. The user interface follows the standard Windows format. The program estimates rates based on structural formulas entered in SMILES³ notation using Taft and Hammett constants for the fragments of the structure. The source for the estimation data is mainly a report to EPA from Stanford Research Institute⁴ as well as a variety of other well-referenced sources. A database of CAS numbers and corresponding structures is also available to permit entry of CAS numbers and retrieval of names and SMILES notation for about 20 000 compounds.

The graphical user interface seems to follow Windows rules most of the time and installation was straightforward. I found little trouble in using the program although in a future release, it would be desirable to set the "focus" to the appropriate button so that once data are entered, calculations could be performed using the "Enter" key or by a mouse click. There are a few idiosyncrasies such as the use of the "PageDown" key to initiate the calculation. Cut-and-Paste

is readily available which makes editing structures or copying results to another application very easy.

Any estimation program such as this one needs to make the user aware when they are pushing the boundaries of the estimation routine or when the program has had to make approximations to deal with structure fragments unavailable in the program. HYDRO does an excellent job of making the user aware of invalid entries, for example, invalid SMILES notation, and of approximations used. I would rate the program excellent on this category and on the format of its output.

REFERENCES AND NOTES

- (1) PC-HYDRO, version 1.50 for Windows, is available from Syracuse Research Corporation, Merrill Lane, Syracuse, NY 13210-4080 (telephone: 315-426-3200). The price is \$400 and the database of SMILES notations with CAS numbers is \$100.
- (2) Windows is a product of Microsoft Corporation, 1 Microsoft Way, Redmond, WA 98052-6399.
- (3) Weininger, D. SMILES, A Chemical Language and Information System. I. Introduction to Methodology and Encoding Rules. *J. Chem. Inf. Comput. Sci.* **1988**, 28, 31–36.
- (4) Mill, T.; Haag, W.; Penwell, P.; Johnson, H. Environmental Fate and Exposure Studies Development of a PS-SAR for Hydrolysis: Esters, Alkyl Halides, and Epoxides. EPA Contract No. 68-02-4256, SRI International: Menlo Park, CA, 1987.

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