Review of ChemKey Search Database for the Macintosh

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The ChemKey Search Database is a listing of more than 40 000 literature references broadly covering organic synthesis: methodology, heterocycles, reactive intermediates, organometallics, photochemistry, asymmetric synthesis, theory, and more. It has been assembled under the aegis of Professor Albert Padwa of Emory University and is marketed by HeteroData of Atlanta. Annual upgrades (ca. 5000 citations) are available at a modest cost. The author/publisher HeteroData, Inc., has occasionally posted a web page through the UCLA Chemistry commercial software listings advertising a free demonstration version of the software as well as the means to order a copy via e-mail.[1]

The program has been reviewed previously,[2] and the current version contains an update of the database itself as well as a reader FileMaker Pro User 2.1v1. It retains its attractiveness in narrow subject coverage and ease of use. These two aspects are inversely related, and the flavor of the database is very much that of the old card file system that graduate students of an earlier era developed during their education and maintained through their active research years. It can only be described as comfortable to have so much information readily available and at no charge beyond initial purchase.

The database and accompanying reader occupy more than 15 Mb of hard disk space. The citations span approximately 25 years, although the pre-1980 entries are quite uneven in their coverage. More than two dozen journals are included—American and International; English language and other; books, standard, communications, and review journal styles. The sources represent a very rich diet of organic chemistry with the emphasis on synthetic methodology but freely mixed with physical and structural information.

Organization of the data is roughly reverse chronological order but changes over time. Records include some or all of the title, journal, journal volume, year of publication, pages covered, a keyword list, and a brief abstract as well as a reference number in the database. Authors' names appeared only if they were part of the keyword listing.

Using the database is simple: The user is presented with a pair of blank boxes to enter search criteria. The first will find textual data (author/ title/keyword); the second finds numerical data. Given a valid and useful term, the search engine will return the first record found along with an indication of the number of "hits", and the option of viewing the records by "flipping through" the stack or "browsing" short forms. The ability to toggle back and forth between these two modes is transparent.

Searching is carried out is by keywords including truncation or clipping, author's names, and "numbers" including year of publication and page numbers. The search engine allows the use of the Boolean "and" and "or" but not the "not"! The records may be viewed in full, one at a time, or "browsed" in a compact format putting 10−15 on a page. Printed output may be expanded to two or four times normal size for production of overheads or slides.

Quality control is problematic: citations are not standard CAS-style citations but a highly individualistic format which changes over time. Early citations do not even include authors' names. The database contains numerous errors of spelling and data entry, for example, "cheletropic", and "Dannheiser" (for Danheiser). Entries are duplicated, and others made with data in the wrong fields of the database or just with the wrong numbers all together. Many entries do not list the authors at all unless their names were put in the keyword list.

Loading the program is quite straightforward since both the database reader and the database itself are equipped with (software) installers. The user is warned to disable any virus detectors on the system before installing, but this operation is common with the installers. The installation is problematical, however. Three machines were tested: a Power Mac 7100/66 (16 Mb RAM, System 7.1.2), a Centris 650 (8 Mb RAM, System 7.1), and a little old Macintosh IIsi (8 Mb RAM, System 7.1). Results were mixed.

The first installation attempt was on the PowerMac. The machine had no active virus-fighting software, but the program would not run (the database would not load properly) after installation. A double-click on the database initiated loading, but the machine would then freeze. A double-click on the reader (FileMaker Pro User) put the machine into an infinite loop. This may be a common incompatibility with the PowerMac architecture.

The second installation was made on the IIsi. Installation proceeded as expected, requiring some 20 min in this case due to the 15-Mb space requirement on the hard drive, and the database came up and seemed to run. Some irregular behavior appeared at intervals, but this was never "fatal" to operation of the program. In one instance, a command to print a record produced 15 pages of citations in the "browse" format. On another occasion, the screen seemed to be stuck on one particular record. Only on the third try, loading the software on the Centris, was installation and operation simple and straightforward.

When running on a system where no printer was active (Centris), an annoying dialog box stating this fact appeared every time a new search was initiated. In one instance, a search produced no hits, but when the "continue" button was used, the database was sorted and presented *in toto*. None of these problems were damaging to either the program or the computer.

The ChemKey Search Database will continue to find users who enjoy its comfortable closure, ease of use, and modest cost. As presented, ChemKey Search is not configured to be edited by the user, but the coverage in its area is thoroughgoing, and, with updates coming does at one-year intervals, the user has only a year's worth of notecards to write as an individual.

REFERENCES AND NOTES

(1) ChemKey Search Database is available form Heterodata, Inc., 1055 Rosewood Drive, Atlanta, GA 30306. Phone (404)727-6586 or 892-4720, Fax (404)727-6629. Internet Chemap@dooleycc.cc.emory.edu. Cost quoted to a graduate student is $475 and $75 for the update.

(2) Pearson,William H. *J. Am. Chem. Soc.* **1993**, *115*(14), 6474.

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