J|A|C|S

COMPUTER SOFTWARE
REVIEWS

ChemKey Search Database. Heterodata, Inc. 1055 Rosewood Drive, Atlanta, GA 30306. http://euch6f.chem.emory.edu/index.html. $325.00.

ChemKey Search Database is a compilation by Albert Padwa and co-workers of 110,000 literature references covering organic synthesis, methodology, heterocycles, reactive intermediates, asymmetric synthesis, theory, and more. He has been selecting key papers from the literature since his postdoctoral work in 1962, joined at times by members of his research group. Although a variety of computer platforms have historically supported this database, in its most recent form, ChemKey uses FileMaker Pro software. The user does not have to own a copy of FileMaker Pro to run the database, as it is distributed with the stand-alone software FileMaker Pro Runtime. Everything that is needed to use the database is included on the installation CD or at the Web download site. An additional 5,000 new citations are offered each year and are available to ChemKey users for importing without charge.

ChemKey Search Database was tested on both a PC and a Macintosh, where a common interface was encountered. The Windows version performs some initial indexing when first used, but once this is done (ca. 30 min), search times are very quick. The Mac OSX version does not require initial indexing.

The database relies on text searching only; there is no provision for structural searches. Query entry is straightforward, using simple instructions that are displayed on the start screen. The database takes only a few minutes to learn to use. Entering a fragment of a search term is sufficient: for example, "ion" rapidly finds all citations containing words beginning with those three characters, such as "ion", "ionic", "ionization", etc. Entering "=ion" finds only ion, whereas entry of "*ion" finds words that contain those characters at any position, including "anion" and "cation". Boolean searches "and" and "or" are also supported. The speed of searches is impressive: with the exception of internal string searches (using *), which may take 30 s or so, all other searches provide results within a second or two, even with multiple search terms. Records may be viewed in full, one at a time, or browsed in a compact format that puts 10–15 references at a time on the screen.

The literature covered by ChemKey includes books and over two dozen journals in organic chemistry. The references are hand-picked and reflect Padwa's broad interests and a distinguished career that spans photochemistry, heterocycles, physical organic chemistry, and especially synthetic organic chemistry. At a minimum, entries include the title of the paper, the name of the journal or book, the volume, year, and page numbers, and the name of the corresponding author. In many cases, an abstract may also be included. ChemKey is not meant to compete with SciFinder, Beilstein, or other on-line chemistry databases; rather, it offers rapid and convenient access to literature that has been selected and characterized by an eminent practitioner of organic chemistry. It is a view of the literature as an organic chemist would see it. One gets Padwa's own judgment about what is significant about each paper, chapter, or book. Thus, each entry bears his imprint as a listing of keywords and perhaps a few sentences about the work. This is clearly one of the most useful aspects of ChemKey—this sort of digestion is not typical of other resources for searching the literature. Beyond Padwa's critical analysis of the literature, another particularly useful aspect of ChemKey is the keyword "review". The database includes a comprehensive set of reviews in organic chemistry, each tagged with this keyword. Further, certain primary literature citations are also tagged in the same fashion if there is a particularly informative overview of the literature by the authors. Thus, in addition to finding traditional books, chapters, and reviews, one might find a hit from a *Journal of Organic Chemistry* paper that has a good overview of the literature in its introduction.

A few examples serve to illustrate the utility of ChemKey. Entering "Julia sulfone" finds references on the Julia olefination, including reviews, specific papers on the development of the Julia olefination, and, significantly, papers where a Julia olefination was a significant aspect of a synthesis. It is clear that Padwa and his co-workers have looked at synthetic schemes and assigned keywords to describe the various reactions that were encountered. Thus, even though the title and abstract of a paper on the total synthesis of a natural product says nothing about a Julia coupling, ChemKey may find several total syntheses where this reaction was employed. For another example, if you want to retrieve key papers rapidly where olefin metathesis has been used to make nitrogen heterocycles, enter "metathesis nitrogen het" and 95 hits will be produced in a second or two in a concise format, showing that various alkaloids and other nitrogen heterocycles have been made with this reaction. In some cases, the metathesis aspect is the subject of the paper, but in other cases, it is simply used in a synthetic scheme—not something that would be obvious in a set of hits from other databases. If you wish to restrict your search to reviews that cover the synthesis of nitrogen heterocycles by metathesis chemistry, enter "metathesis nitrogen het review" and you will find five reviews, including one on the construction of alkaloids with ring-closing metathesis and two others that specifically focus on making nitrogen-containing heterocycles with ring-closing metathesis. Since the database searches all fields simultaneously, if you recall the last name of the corresponding author, you can quickly find what you need. For example, if you are interested in the gem-dimethyl/Thorpe–Ingold/reactive rotamer effect and recall that Jung did some nice work in that area, type in "Jung gem review" or something similar and you will quickly find his 2005 article in *Chemical Reviews*.

In summary, ChemKey Search Database is simple and fast to use, does not require an expensive subscription to an on-line database, and exists right on one's desktop computer. Its primary benefit is the rapid retrieval of key literature entry points for a given subject or author. The critically selected citations, chosen

by an expert organic chemist, are obviously selected with the practicing organic chemist in mind. The database is not meant to be comprehensive like some of the other tools that chemists use, so one may not find all of the references on a given topic. However, the user is not overwhelmed with hundreds of hits to sort through; the hits that appear have been carefully selected and provide a useful entry point to the literature on a given subject. In many cases, coauthors are missing and the paper's title and abstract are paraphrased, so if a truly comprehensive literature search is required, more traditional tools must be employed. ChemKey is for the rapid retrieval of predistilled organic chemistry literature.

Overall, this is an excellent product that provides a convenient means for rapidly searching the organic chemical literature at a very reasonable price. It is a useful complement to more complex, expensive, and comprehensive search tools. Padwa and his co-workers are to be commended on making this resource available and for continuing to provide yearly updates free-of-charge.

William H. Pearson,
Berry & Associates, Inc.