

a Compaq 386/25, IBM AT, Epson Equity 286/12, and a number of no-name clones. I had no trouble with any machine I tried. Only my wrist tired after loading all the floppy disks! The system comes with a 29-page manual and a 10-page Appendix A, which consists of a good set of examples. I would rate the technical information and accuracy of the manual as high.

As for searching the database, the system is quite easy to use and rates a good grade in the area of user friendliness. Searches for CAS Registry Numbers, ID numbers, and molecular formula took less than a second of elapsed time. The hyphens in the CAS Registry Numbers are not needed in a search; in fact, if one tries to enter a hyphen, the program will not allow it. I like features like that "know" enough to let you enter something in more than one way and still get the right answer. A molecular weight search took from 1 to 3 s depending on what, if any, constraints were placed on the search. The slowest search in the system, a sequential search of the entire database using 10 peaks, took about 4.5 min with the CD-ROM version using a Epson Equity 286/12 with a 40MB hard disk operating at a clock speed of 12 MHz and only 65 s on a Compaq 386/25 with a 110 MB hard disk.

This latest version of the system comes with the option to create and maintain a private database of mass spectral data, which is the "User Database" option. The user manual describes how this is done quite well and no one should have any trouble creating their own local database. Thus one can search either the master database, a private local database, or both. Of course the private database created will be on your hard disk, not on the CD-ROM.

At present there still are no plans for a Macintosh version of the system. Substructure searching of the entire database on the PC is probably not too far away. All in all, this is a

very impressive, well-designed system, and for the low cost, this should be bought by every mass spectrometry or organic chemistry laboratory and organic chemical spectroscopy course. Useful, easy-to-use databases for the PC (and hopefully the Macintosh too) are the wave of the future. See the future now by getting this database and learning how to make effective use of it. It surely will be followed by many others like it in the next few years.

REFERENCES AND NOTES

- (1) The database is available either on floppy disks or CD-ROM. The system program written by Dr. Stephen E. Stein, National Bureau of Standards, Office of Standard Reference Data, Building 221, Room A-325, Gaithersburg, MD 20899. The database on floppy disks is available from NIST, OSRD, Physics Building, Room A323, Gaithersburg, MD 20899 for \$1050.00. The same database on a CD-ROM is available (catalog no. Z21,399-3) from Aldrich Chemical Co., 1001 West Saint Paul Ave., Milwaukee, WI 53233 also for the same price of \$1050.00.
- (2) Heller, S. R.; McGuire, J. M.; Budde, W. L. *Environ. Sci. Technol.* **1975**, *9*, 210.
- (3) Heller, S. R.; Milne, G. W. A. *EPA/NIH Mass Spectral Data Base*, in five volumes, part of the NBS' National Standard Reference Data Series of Critical Data Compilations (GPO no. SN003-003-01987-9, NSRDS-NBS 63), 4634 pp., U.S. Government Printing Office (1978 and reprinted 1980).
- (4) Heller, S. R.; Milne, G. W. A. *EPA/NIH Mass Spectral Data Base, Supplement Number One*, in two volumes, part of the NBS' National Standard Reference Data Series of Critical Data Compilations (GPO no. SN003-003-02268-3, NSRDS-NBS 63, Suppl. 1, 2151 pp, Dec 1980).
- (5) Heller, S. R.; Milne, G. W. A.; Gevantman, L. H. *EPA/NIH Mass Spectral Data Base, Supplement Number Two*, in two volumes, part of the NBS' National Standard Reference Data Series of Critical Data Compilations (GPO no. SN 003-003-02268-3, NSRDS-NBS 63, Suppl. 2, 1110 pp, 1983).
- (6) Heller, S. R. NBS Mass Spectrometry Database. *J. Am. Chem. Soc.* **1988**, *110*, 3336-3337.
- (7) Dillard, J. G.; Heller, S. R.; McLafferty, F. W.; Milne, G. W. A.; Venkataraghavan, R. *Org. Mass Spectrom.* **1981**, *16*, 48-49.

Pro-Search, Pro-Cite, and Biblio-Links

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More and more chemists are involved in online searching of databases and management of the ensuing results, but if they are like me, they don't enjoy it very much. The collection of programs from Personal Bibliographic Software Inc. (PBS), which are reviewed here, helps to alleviate much of the tedium of database searching and management of results. To accompany the programs, PBS also publishes *Format*, a quarterly newsletter, free of charge.

Pro-Search¹ is a program which acts as a front-end to online services, such as DIALOG and BRS. It simplifies searching for the novice and helps the experienced user. There are a number of other similar programs, such as STN Express and DialogLink, but Pro-Search has the advantage of being one of a series of programs from a single vendor. It suffers from the disadvantage that is tailored to the overall bibliographic market, while a program like STN Express is more oriented to the chemical, scientific, and technical community.

Pro-Cite² takes the properly converted search results and converts the bibliographic references into a form that allows the information to be used readily in bibliographies. Finally, Biblio-Links^{3,4} is a set of programs that serve as the interface between Pro-Search and Pro-Cite and allow one to convert Pro-Search literature search results from a variety of online

systems into the format used by Pro-Cite, after they have been downloaded to the hard disk.

Each of the three programs can be purchased separately for IBM PC or Macintosh computers. Copies of all three were available for my IBM PC, and so this review will cover all three programs, using the STN and DIALOG modules as examples of the Biblio-Links programs. All three programs can be ordered on 3 1/2 in. or 5 1/4 in. disks. The programs all require varying amounts of storage; with all the options installed, Pro-Search and Pro-Cite, the two largest, each require about 1.3 Mbytes. Each Biblio-Links module requires 0.15 Mbytes of disk storage. The programs require DOS 3.0 or higher and only 320K of RAM. A color monitor is optional. Installation is easy, but the manuals are somewhat confusing. The installation of Pro-Search, for example, is made unnecessarily difficult by the need to skip around the manual depending on a variety of parameters. The first 100 pages of the Pro-Search manual deals with installation and only then does one find the Table of Contents. I installed Version 1.08 (dated October 1989), but if you wish to upgrade to 1.08 starting from 1.03, 1.04, 1.05, or 1.07 (whatever happened to 1.06?), a slightly different procedure must be used. With the advent of easy-to-use install programs such as the one supplied

with WordPerfect 5.1, this seems to be behind the state of the art. As it turned out, I had to call the PBS help desk to overcome a few minor programs that should not exist. Once I got over the installation hurdle, however, the programs worked just fine.

Pro-Search most resembles DialogLink in operation. In setting up the program, one enters the phone number, account number, and password for the system(s) one plans to access. This makes subsequent login a breeze and since search queries are prepared offline, searching can begin immediately after login. A feature in Pro-Search allows the use of the same menus for searching DIALOG or BRS, and it is even possible to search in DIALOG with BRS commands and vice versa. Assuming one can afford hard disk space (and the quarterly updates) one can store all the DIALOG Bluesheets so they can be accessed at any time. The program operates in either of two modes, Native and High-Level. In the Native mode, one sees what one is used to seeing when logging into an online system. In the High-Level mode, one can search both BRS and DIALOG with the same set of on-screen commands, and the program provides a combined BRS/DIALOG subject catalogue. As a chemist, I saw few reasons to use this option and so, beyond testing it to see if it worked as advertised (it did), I did not use it. Pro-Search suffers from being a little outdated in its user interface. For example, no list of function key functions is printed anywhere on the screen; to access this information, one must hit F1, then type H, then O. A single keystroke would be much more convenient. But all in all, Pro-Search is a good program, and it should prove useful to most online searchers.

The second program, Pro-Cite, is used after Pro-Search to help manage bibliographic records. It can also be used by entering records manually and using one of the Biblio-Links programs described below. The version of Pro-Cite that is reviewed here is 1.41. An update to this version is expected by mid-1991. Installation of Pro-Cite is very straightforward, although a bit cumbersome. The setup program is not very forgiving of errors, nor does it let you back up one step if you make a bad choice. Choosing the foreground and background, for example, is a two-step process, but if you choose a foreground which when you see the choices of the background you realize is wrong, then you have to rerun the entire setup program. You can not stop and exit from the setup program after you realize you don't like something you did. As setup is easy to rerun; however, these are minor problems.

Pro-Cite comes with 20 predefined work forms for storing a record in different ways. In addition one can define one's own work form of data structure formats. The system allows for up to 32 000 records, and each record can contain as many

as 16 000 characters, so abstracts of virtually any length can be handled by the system. Pro-Cite, as distinguished from database management systems such as dBase, has a variable record length capability, so its storage requirements are kept to a minimum. The Pro-Cite editor is quite adequate for entering and modifying records, and records can be sorted on one or more fields. Duplicate records are automatically detected, and you can select the one you want to delete. One modern user interface feature that is missing here is that while one can retrieve and use a file from any disk directory, it is not always possible to specify where the results will be stored; the results are always put back in the directory from which they came. Thus if one does a search with Pro-Search, reads the file into Biblio-Links and then into Pro-Cite, one cannot store the file in the Pro-Cite directory without leaving the program and using the DOS copy command to put the Pro-Cite files in the Pro-Cite directory. In spite of such minor shortcomings, this module is very popular and very widely used, and I would recommend it. As an example of its use, the excellent book in chemical information, *Chemical Information Sources* by Gary Wiggins⁵ comes with a Pro-Cite-generated computer-readable file, called the Chemistry Reference Sources Database, which contains over 2150 records of references from the textbook.

Biblio-Links, the companion module to Pro-Cite, is a widely used program which converts bibliographic references into a form Pro-Cite can handle. This program examines a downloaded search results file, extracting the fields for the previously defined Pro-Cite work form or your own custom format. Both the DIALOG (version 3.0) and STN (version 1.0) versions of the Biblio-Links programs worked smoothly when tested with small files from a simple search.

REFERENCES AND NOTES

- (1) Pro-Search is available from Personal Bibliographic Software Inc., P.O. Box 4250, Ann Arbor, MI 48106. The price of the complete program (IBM PC and clones) is \$495.00. Upgrades are available for \$150.00 per year. There is also a Macintosh version.
- (2) Pro-Cite is available from Personal Bibliographic Software Inc., P.O. Box 4250, Ann Arbor, MI 48106. The price of the complete program (IBM PC and clones) is \$395.00. There is also a Macintosh version.
- (3) Biblio-Links modules are available from Personal Bibliographic Software, Inc., P.O. Box 4250, Ann Arbor, MI 48106. The price of each module is \$195.00. Reference 4 lists the modules available for the IBM PC and clones. The first three (asterisked) are also available for the Macintosh.
- (4) The currently available modules for Biblio-Links are: BRS*, DIALOG*, MEDLARS*, OCLC, SilverPlatter, STN, NOTIS, US-MARC, DGIS, DROLS, DOBIS, MUMS, and SCORPIO. According to the vendor, the BRS Biblio-Links version (3.2 or higher) can be used to transfer ORBIT records into Pro-Cite.
- (5) Gary D. Wiggins. *Chemical Information Sources*. McGraw-Hill: New York, 1991.

The PESTICIDES Disk

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In the field of chemistry alone, one could spend a lifetime in the thorough review of information sources. When one adds biology, economics, and survival (i.e., agriculture) to the mix, the dimensions of the information problem grow factorially. Such is the domain of pesticide information. Chemistry in every form, shape, and fashion may be involved. Physical

properties, synthesis, degradation and breakdown, transport, biochemical impacts, and so on, all may be key elements in both scientific or practical queries. Information about a selected problem/pest, of what crop, in what geographic region, with what soil/ecologic/cultural/economic factors present at what levels define possible vectors for searching. Concerns