

ChemLink Fine Chemicals Database on CD-ROM[†]

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This review and the following one on the Aldrich CD-ROM database of material safety data sheets are the start of the first commercial CD-ROM (compact disk—read only memory) products to come whose content is primarily for chemists. While there are a few hundred CD-ROM disks now available, most are used either for in-house purposes (e.g., manuals or catalogs) or for library needs (e.g., Books in Print).

The ChemLink Fine Chemicals Directory is a database and associated software put onto a CD-ROM that contains the chemicals being sold by 31 suppliers from 6 countries. While one can get all the 31 catalogs (and many more) for nothing, having them in an easy to use form is useful, convenient, and worth something. The ChemLink product comes with a CD-ROM disk that contains the database and a floppy disk with the FindIT software. The FindIT software is a "shell" CD-ROM search package that a number of CD-ROM packages use. The FindIT Users Manual and Installation Guide is very generic and provides little help when a specific problem arises. Installation was a minor problem, as I did not have the latest (version 2.0) CD-ROM drivers for my IBM-PC and Amdek/Hitachi CD-ROM reader. So \$28 poorer and a week later I installed the system on my IBM-PC (an IBM AT with 640K, a 30-MB hard disk, and a 40-MB Plus Hardcard). The installation went fine once I agreed with the FindIT software to only use drive C. While the software said drives D and E were OK to use, it was quite clear the programmer who wrote the installation routine was either kidding or never tried to install the system on anything but drive C. (Actually the software did install the system on drive D, but created a subdirectory whose name looked like Chinese or Martian hieroglyphics, and not having the foggiest notion of what ASCII code corresponded to this subdirectory name, I surrendered and allowed the system to go on drive C.) However, within 2 weeks after reporting this bug to the vendor, I was sent a new installation disk that corrected the problem. Since then I have not found any more bugs.

The database has some 137 020 records or entries (including duplicates) from the 31 suppliers. The database can be searched in nine different ways: by (full) chemical name;

chemical name fragment (37 606 different entries); CAS Registry Number (available in 28 350 different entries); molecular formula (25 427 different formulas, but not every record has one); molecular formula fragments (986 different fragments); element fragments or element symbols (of which there are 83 of the 103 elements); supplier code name (of which there are 31 suppliers); supplier country (of which there are 6); and a catch-all field called "All Fields". The last one is quite convenient for searching using the Boolean logic available.

It is difficult to say much about the system. It simply is a very nice and easy way to search and see if a particular chemical is available for purchase and get the detailed record(s) from the chemical catalog(s) that have the chemical wanted. Searches are easy to perform, and hard-copy printout is a readily available option. It is easy and fun to browse through the database. User support is good. Telephone calls for help were returned within a short period of time. Having a User's Manual should be a feature included for the next release. The system comes with a FindIT User's Manual, but this manual is highly generic for all CD-ROM databases that use the FindIT software. The ChemLink system is case sensitive, but I found that out only by talking with the system developer from ChemLink, after indicating certain searches did not seem to work. The price of \$450 is very reasonable for a CD-ROM product that is not likely to sell a large number of copies too soon, as few chemists or labs have CD-ROM readers. I would think every chemistry department laboratory stockroom should have ChemLink. It is certainly cheaper to use than the online ORBIT ChemQuest product, though it presently does not have as many entries or suppliers. For chemical or science libraries that already have a CD-ROM reader, ChemLink is a worthwhile addition to a CD-ROM collection. As time goes on and more chemists get CD-ROM readers for their PC's, the cost of a CD-ROM reader now being in the neighborhood of \$700–\$900, products like ChemLink will become more popular.

In summary, for the first release, ChemLink is useful, reasonably priced, easy to use, and a worthwhile database to have for any chemical group that needs to order laboratory research chemicals.

[†] Available from Chemron Incorporated, 3038 Orchard Hill, San Antonio, TX 78230-3057 [(512) 493-2247]. \$450.00, not including CD-ROM reader.

Sigma-Aldrich Material Safety Data Sheets on CD-ROM[†]

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This is the first CD-ROM database from Sigma-Aldrich Chemical Co., an innovative supplier of chemicals and related data and information on the materials they sell. Aldrich has

published books of spectral data (IR, FT-IR, and CNMR) and now has moved aggressively into the developing market for material safety data sheets (MSDS) and other databases. The database of Aldrich MSDS contains some 30 000 MSDS with chemical structures. The database is updated every 3 months. The system is available for both the IBM-PC (and its clones) as well as the Apple Macintosh computer. The

[†] Available from Aldrich Chemical Co., P.O. Box 355, Milwaukee, WI 53201 [(414) 273-3850; FAX (414) 273-4979]. \$1300 per year (catalog Z17,500-5), not including CD-ROM reader.

system reviewed was the IBM-PC version, release 2.10.

The system comes as one CD-ROM disk and two floppy disks. One floppy disk is for the search software, and the second contains the printer drivers. The system requires an IBM-PC or equivalent, using DOS 3.1 or higher, and at least 512K of memory. A printer and a hard disk are desirable, but not mandatory. The current software release (version 2.10) cannot take advantage of a color monitor. The 18-page, 4-in. by 4-in., instruction manual is good, and there was no problem installing the system. The trouble-shooting section indicates five common system error messages and mentions a few bugs still left in the system. In doing some sample molecular formula searches, I found the system froze my computer a number of times as the buffer overflowed into areas of memory, which causes the system to stop running. This is a bug that needs to be fixed soon.

The system can be searched by complete chemical name, CAS Registry Number (CAS RN), Aldrich/Sigma product number, and formula. No partial or fragment name searching is available now, but is currently under development. Printing of a single MSDS or a series of MSDSs as well as a simple online help screen is available. Chemical name, product number, and CAS RN searches were simple to do. The search times were slow, on the order of 5 s, but typical for a CD-

ROM. The browsing capabilities of the CD-ROM FindIT software (described in the previous review on the ChemLink CD-ROM product) are also being added to the system and will be released later in 1989. The current graphics software does not allow for a blinking cursor, and this, too, is annoying since the user is not sure where he/she is on the screen.

The quality and quantity of the data are considerable. Compared with the J. T. Baker and Mallinckrodt MSDS databases on floppy disks, which have only some 1400–1600 compounds and cost about the same amount of money, this is a large database of MSDS information. As expected, actually converting all of the MSDS data for about 15 000 compounds into a very useful form (i.e., a CD-ROM) tends to quickly show the developers, and the users, what additional housecleaning is needed to be done to the database. To their credit, Aldrich is working hard at these problems, and from what I have seen from the one update I received, they are making headway. This CD-ROM MSDS database is probably one of the best available, has a large number of chemicals in the database, and is reasonably priced. Being in the business of selling chemicals, there is no question that Aldrich is here to stay. Thus, it is expected that improvements will make this an even better product as time goes on.