Computer Software Reviews

ChemQuest. Database producer: Molecular Design Ltd.: 2132 Farallon Drive, San Leandro, CA 94123; 415-895-1313 or 800-MDL-0064 outside of California. The size of the file is over 210 000 records, updated quarterly. Chemquest is available for online searching through both Pergamon Financial Data Services (PFDS) Achilles House, Western Avenue, London, England W3 OUA, or ORBIT Search Service, 8000 Westpark Drive, McLean, Virginia 22102.

For practicing chemists, the question often arises whether it is necessary to make the compound that is needed for the next step in ones work. For an easy answer to the question "can I buy it?" there is an online database called ChemQuest that is accessible through such telecommunication networks as Telenet, Tymnet, or Datapak.

ChemQuest is a database of over 91 000 compounds available from the leading international chemical suppliers in the US, Europe, and Japan. You can easily search over 60 chemical catalogues simultaneously and find suppliers, quantities, and prices for the chemicals you need. The database covers sources of organics, biochemicals, dyes, stains, and some inorganics as well. There are however some useful catalogues that are not included, for example those from Merck, Sharp & Dohme/Isotopes, listing many ^{2}H- and ^{13}C-labeled compounds, and the Roth natural substances catalogue. Perhaps these can be included in future updates.

ChemQuest has two types of searching modes, text and graphics. The basic equipment needed for text searching is any standard TTY terminal and a modem (capable of handling 1200 or 300 baud). For searching by structure, a graphics terminal (such as Tektronix, Westward, Sigma, DEC VT640, or Pericom) or a personal computer with emulating software is required (for instance Versaterm for the Macintosh or Emu-Tek for IBM compatibles).

In the text searching mode one can search for compounds by name, molecular formula, or CAS registry number. The exact name of the chemical, as it appears in the catalogue, must be used in order for it to be retrievable. Unfortunately, addendums such as purity are presently included in the exact chemical name. Therefore CAS registry number would be a more useful tool for searching in text mode. However, not all catalogues include it although the major ones do. This means that not all compounds in the database have an associated CAS registry number. Addition of these numbers for all compounds in the database is underway. One can also use name truncations and name fragments with Boolean search operators to avoid having to enter the name exactly. Searching by structure or substructure is done in the graphics search mode.

Searching by structure is often the most convenient search mode, saving the extra work involved in guessing the correct name or finding the CAS registry number. After entering the terminal type the user is confronted with a main menu. This menu allows the choice of various search options, such as structure search, substructure search, in addition to CAS registry number, formula, or name search. It is also possible to make a list of preferred suppliers before the search in the main menu. (ChemQuest Handbook provides a complete listing of ChemQuest suppliers, their addresses, phone and fax numbers, as well as their agents worldwide. Listprice for the handbook is $35.00.) Any of these options can be selected with the aid of the cursor (cross-hairs) and "pressing the button". To activate the option, the cursor is placed over the choice and either a space bar or a mouse button is pressed or a lightpen is used. When doing structure or substructure searches the structures are entered on a sketchpad very similar to that in use in the ORAC or LHASA programs.

The structure sketchpad consists of three major parts; the blank drawing area, templates on both sides of the drawing area to facilitate drawing of structures, and across the top, a list of the various command options, such as move, erase, shift, save, recall, delete, search etc., altogether eleven commands. The templates contain structures which ChemQuest will automatically draw or place when instructed to do so. Templates allow rapid entry of rings, atoms, and other common structural units occurring frequently in chemical structures. The structure is built by using the cursor for making bonds or rings not offered in the templates. The cursor is used as a "pen" to draw the required structure. First the starting point of the bond is positioned and activated by pressing the space bar. The cursor is then moved to the next atom position and activated again. A single bond will appear between the two positions. Another bond will be drawn each time the cursor is moved and activated. The drawing of structures is easily learned, and after becoming familiar with it one tends to prefer it to other search modes.

Once the structure is drawn, an on-line search is completed in seconds. A successful search allows the user to browse through the catalogue entries of all suppliers that stock the corresponding structure. If there is no commercial source found for the target structure, it is very easily, just by pushing the button, transferred to the substructure sketchpad for modifying the structure if one wants to continue the search. In the substructure mode any nondesignated atom is assumed to be carbon. Thus all hetero atoms should be specified or labeled by a "wild card" atom X which can be defined as various atoms. The substructure mode is even more valuable than the exact structure searching because by searching analogues one may find new interesting, perhaps more useful or less expensive alternatives to the original starting material.

One of the unique features of ChemQuest, online Ordering Service, has unfortunately been discontinued on all online services and Molecular Design Ltd. has no plans to reinstate it.

The Fine Chemicals Directory, ChemQuest, is now available in three different formats. It is available as an online database from two different online services, Pergamon Financial Data Services (PFDS) or through ORBIT Search Service. An annual fee of $35.00 is charged for a userid and password by ORBIT. The charge for the use of ChemQuest itself is on the basis of connect time, $115 per hour by ORBIT Search Service (January, 1989) and $130 per hour by Pergamon Financial Data Service (May 1989). However, there is a $15.00 (ORBIT) or a $18.50 (PFDS) minimum charge on each monthly invoice issued. If the service is not used in a given month there is no charge. No extra charges are made for displays and there is an offer of 30 min free connect time for new users. There is also a help desk available in both Services. The second format of ChemQuest is the Fine Chemicals Directory, formatted for use with the mini- or mainframe software systems MACCS-II and REACCS, from Molecular Design Limited. Finally in Europe, magnetic tapes of the ChemQuest database are available from Fraser Williams (Scientific Systems) Ltd., London House, London Road South, Poynton, Cheshire, SK 12 1YP, UK.

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