

The Retrieval & Dissemination of
Chemical Information. IV.
ICRS *RADIICAL* Software.

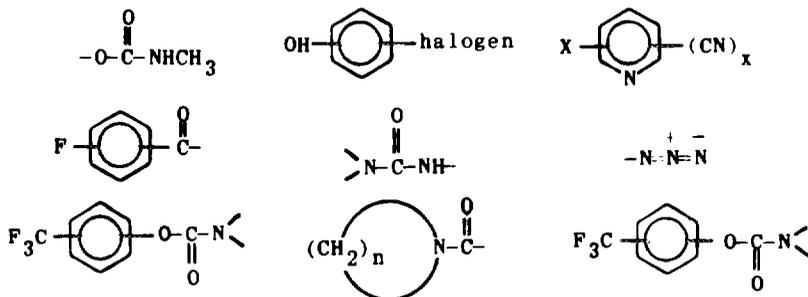
August 5, 1970

Software is a major problem for any organization that uses a computer. To derive full benefit from their computers, some organizations maintain experienced systems analysis and programming staffs. Others utilize various commercially available "packaged" programs. Packaged programs for computer applications such as payroll, inventory, billing, etc., are plentiful, but not for chemical information systems. This problem was fully considered when ISI[®] developed its *Index Chemicus Registry System*[®] (*ICRS*[®]), discussed in previous editorials.^{1,2,3} Every *ICRS* subscriber receives a set of computer programs designated *RADIICAL*[™] (Retrieval and Automatic Dissemination of Information from *Index Chemicus*[®] and Line Notations).

RADIICAL programs are designed to effectively search the *ICRS* tapes, which cover the approximately 50,000 abstracts published each year in *Current Abstracts of Chemistry and Index Chemicus*[™] (*CAC&IC*[™]). These abstracts report about 200,000 new compounds each year. *RADIICAL* programs combine the advantages of special screening techniques⁴ with a string search logic.⁵ They are written in Assembly Language Programming (ALP) for an IBM 360 system (30 or greater), with DOS and OS versions available.

RADIICAL programs can be used to perform searches on article titles (for words, word fragments, word phrases, or word combinations), *subject terms* (supplied by ISI chemists), *use profiles* (applications for which reported compounds were tested), *analytical codes* (analytical techniques used by the authors for the research reported), *authors*, *organizations*, and *substructures*.

Of these capabilities, substructure searching is probably the most useful to chemists. For example, using *RADIICAL* software, substructure searches for compounds containing the following fragments can be performed:



This substructure search capability is invaluable in such applications as compound inventory control, structure-activity studies, and many others.

In addition to their use with *ICRS*, *RADIICAL* programs can also be used to search other data files. With no alteration whatsoever, *RADIICAL* programs can be used to search *ISI Source* and *Citation* tapes. Thus, if an organization subscribes to *ICRS*, it will already possess useable software compatible with these other *ISI* tapes. If the *ICRS* subscriber also constructs tape files covering his own compounds, the *RADIICAL* programs can also be used to search them. (Naturally, any existing tapes might have to be reformatted to make them compatible with the *RADIICAL* programs. This has been done in many organizations.)

Even if your organization were prepared to spend \$50,000 to \$100,000 to prepare a similar set of programs, it might not be possible to obtain a number of unique features included in the *RADIICAL* system. Yet, *ICRS* subscribers obtain *RADIICAL* programs without any additional charge. The software cost savings alone could more than justify the cost of the *ICRS* subscription. Furthermore, *ISI's* computer professionals set up the *RADIICAL* programs in the subscriber's computer center to insure an operational system. This service is also provided without additional charge.

The total annual cost of the *ICRS* system is \$9500 per year for tapes, printouts, *RADIICAL* programs, and professional back-up by *ISI* chemists, information scientists and computer personnel.

1. Garfield, E. The retrieval & dissemination of chemical information. *Current Contents*[®], No. 28, July 15, 1970, pp. M1-2.
2. Garfield, E. The retrieval & dissemination of chemical information. II. The Wiswesser Line Notation. *Current Contents*, No. 29, July 22, 1970, pp. M1-2.
3. Garfield, E. The retrieval & dissemination of chemical information. III. The *Index Chemicus Registry System*[®] (*ICRS*[®]). *Current Contents*, No. 30, July 29, 1970, pp. M1-2.
4. Granito, C.E., et al. "Computer-generated substructure codes (bit screens)". Presented in part at the MARM Meeting in Newark, Delaware, April 1, 1970.
5. Garfield, E., et al. *Index Chemicus Registry System*: pragmatic approach to substructure chemical retrieval. *J. Chem. Doc.*, 10(1), 54-58 (1970).