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Research Information at ICI United States†

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The Research Information Section at ICI United States provides background for planning and carrying out the ICI United States chemical and biomedical research programs and supplies technical information to nonresearch units. Information is furnished in the forms of retrospective literature studies, current awareness bulletins, computer-produced bibliographies, and reports of internal research data. On-line services used include MEDLINE, TOXLINE, CHEMCON, and PATS. Current awareness includes a current chemical literature system based on CA Condensates and Central Patents Index, a computerized biomedical literature system with selection from both primary and secondary sources, and a chemical market and business information system based on Predicasts' Chemical Market Abstracts tape.

The Research Information Section at ICI United States provides background information for planning and carrying out the ICI United States chemical and biomedical research programs and supplies technical information to nonresearch units. Information is furnished as retrospective literature studies both large and small, as current awareness bulletins, and as reports of internal research data.

Our organized information effort for the research program began in 1956 with the establishment of the Information Branch of the Chemical Research Department of Atlas Powder Co.[1] In 1959, it became the Research Information Section of the Chemical Research Department and in 1970 became part of the Research and Development Department. Atlas Powder Company changed its name to Atlas Chemical Industries in 1961, and, in 1971, Atlas Chemical Industries was acquired by ICI Ltd., first becoming ICI America Inc., and, in 1974, ICI United States Inc.

ICI United States has broad interests including polyols, surfactants, textile chemicals, dyestuffs, activated carbon, plastics, and pharmaceuticals.

The Research Information Section presently consists of 14 professional and six clerical employees; the Manager reports to the Vice President and Director, Research and Development. Of the professional employees in Research Information, there are six with Doctorates, three with Masters, and five with Bachelors degrees. The education of ten of the staff is primarily in chemistry and four primarily in biology.

The Research Information Section and the corporate library are separate units but are located adjacent to each other. The corporate library, which serves the entire company, is the major source of information for the Research Information Section.

Most of the work of the Research Information Section is carried out on projects related to those of the ICI United States Chemical Research, Biomedical Research, Clinical Research, Chemical Engineering, and Product Development Departments. Its program is developed annually in support of and in conjunction with these departments. Other functions of Research Information include patent liaison between these departments and the Patents and Licenses Department, and liaison in the exchange of scientific and technical information between ICI United States and divisions of ICI Ltd.

RETROSPECTIVE LITERATURE STUDIES

Specific knowledge of the state of the art of each element of the research program is required for its planning and to support its progress. The Research Information Section collects, organizes, and summarizes what is known about prospective and on-going areas of investigation.

The results of these literature studies are reports which may range from comprehensive reviews through shorter

† Presented in the Symposium on Information Groups in Chemical Companies—Services, Special Systems, and R&D, 9th Middle Atlantic Regional Meeting of the American Society, April 24, 1974, Wilkes-Barre, Pa.

Bulletins from CA Condensates	Bulletins from Central Patents Index
Analytical Chemistry	
Physical Chemistry	
Organic Chemistry	Organic Chemistry
Polymer Applications	Polymer Applications
Polymer Chemistry	Polymer Chemistry
Foods, Pharmaceuticals, Cosmetics, Agricultural Chemicals, Activated Carbon	Foods, Pharmaceuticals, Cosmetics, Agricultural Chemicals, Activated Carbon
Textile and Industrial Chemicals	Textile and Industrial Chemicals

Figure 1. Chemical current awareness bulletins.

studies to the determination of novelty of proposed compounds, processes, and uses. Examples of extensive surveys include a review of the chemical nature of the surface of carbon to support our research program on activated carbon and a review of the mechanism of interaction of surface active agents with components of flour to provide a basis for development of food additives. Such reports involve selection of relevant literature, critical evaluation of the information contained therein, application of imagination, and awareness of project and program objectives. Thus, frequent contact between information and laboratory research personnel and with research management is essential. Longer surveys are usually planned in advance as part of the Research Information Section program; provision also is made in the annual budget and program for shorter studies to obtain information to support the several elements of the ICI United States research effort. Most of these shorter studies are to determine whether proposed substances, reactions, or uses are novel. Research proposals are made by information scientists either as part of their literature studies or separately.

The ICI United States new drug research effort is organized into teams in each therapeutic area; there is a member from Research Information on each new drug team as well as members from Medicinal Chemistry, Pharmacology, Safety Evaluation, and Clinical Research. The information representative on each team studies and reports the relevant chemical and biological literature to help develop the program and to provide the informational basis for selecting drug candidates and testing methods. The information representative also helps evaluate research suggestions and participates in team recommendations to the Biomedical Research Department management.

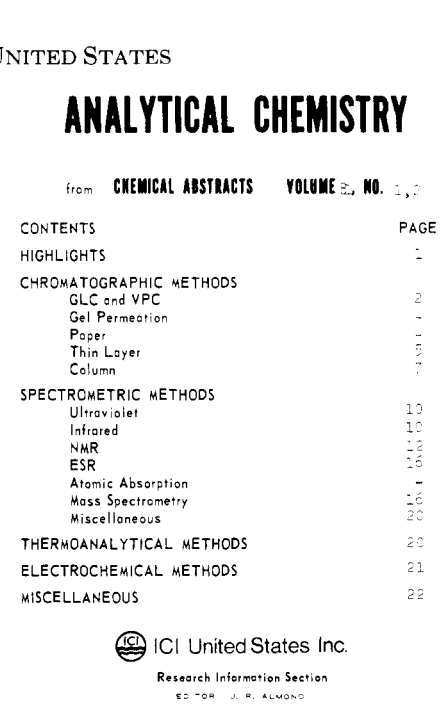
Not all studies are directly related to the research program. For example, information is obtained for personnel in nonresearch units of the company on identity and characteristics of new materials and processes, on properties of proposed raw materials, on manufacturing procedures, on toxicity of specific chemicals and classes of compounds, and on environmental matters.

The sources of information used for our retrospective literature studies include reference books, journals, patents, trade publications, and internal reports. Recently we have found the on-line services of MEDLINE, TOXLINE, CHEMCON, and PATS[2] to be particularly useful for rapid identification of relevant literature, or to furnish specific information, or both. We expect our use of on-line services to increase.

CURRENT AWARENESS

Information about current publications relevant to our research programs and to ICI United States products is disseminated in current awareness bulletins covering our chemical, biomedical, and chemical market interests. Distribution is only to company personnel.

We believe that each scientist is interested not only in specific topics of concern to his own work, but also in tangential areas in the same general field. Accordingly, our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Research Information Section
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Figure 2. Cover page of *Analytical Chemistry* bulletin showing subdivisions.

current awareness dissemination is by subject area bulletins, rather than by individual SDI.

Our current chemical literature system[3] is based on CA Condensates and Central Patents Index. The 12 subject area bulletins which make up the system are indicated in Figure 1. Each bulletin is published biweekly.

The bulletins are further divided into subject areas as shown by the cover page of *Analytical Chemistry* (Figure 2). Selection of material for the bulletins from the CA Condensates tape is by 157 profiles, of which 93 are for the odd issues (including Organic Chemistry) and 64 are for the even issues (including Macromolecular, Applied, Physical, and Analytical Chemistry). Selection from Central Patents Index is by direct inspection of the Derwent Basic Abstracts Journals or the Alerting Bulletins. Preparation of profiles and selection of articles or patents for inclusion is carried out by five members of the Research Information Section, each of whom edits two or more bulletins. The bulletins derived from CA Condensates consist of abstracts from *Chemical Abstracts*. In the patents abstract bulletins from Central Patents Index, if available, basic abstracts are used in preference to the alerting abstracts because they supply more information. The pages of each bulletin with abstracts are also order sheets which can be used to request an article or to obtain a copy of a patent. Each bulletin includes a highlights page in which articles or patents of particular interest are indicated. About 15,000 articles and 7,000 patents are cited in the chemical bulletins each year.

Collection, analysis, and dissemination of information about current publications related to our pharmaceuticals interests involves the computerized Atlas Biomedical Literature System (ABLS).[4] This system provides both current awareness as well as the storage and retrieval of biomedical literature of interest to our research program or our marketed drugs.

After analysis of an article, descriptors are assigned from a controlled vocabulary. The bibliographic data for each article and the descriptors are referred to collectively as a condensate. Currently contributions to the ABLS are made by six Research Information Section personnel. Information about current published articles is disseminated in the semimonthly Biomedical Condensates, which is primarily concerned with our preclinical program, and the weekly Pharmaceutical Condensates, which covers published articles related to our clinical research interests and the mar-

Surfactants, Fine and Specialty Chemicals and
Activated Carbon
Plastics
Textile Chemicals and Dyestuffs
Fertilizers and Agricultural Chemicals
Industrial Chemicals and Miscellaneous

ins

Figure 3. Current chemical market abstracts bulletins.

keted drugs of our Stuart Pharmaceuticals Division. About a third of the condensates which are entered on tape are published in the two current awareness bulletins. In selecting literature related to our preclinical program, greater emphasis is placed on the physiological, biochemical, and pharmacological phenomena involved rather than on specific drugs. In support of marketed drugs and for our Clinical Research Department, we report articles on specific ICI United States drugs, on prospective drugs, on important competitive products, adverse reactions, diagnosis, pharmaceutics, and analysis. Articles are entered in the ABLS, both to furnish information during drug development to the ICI United States personnel involved, and to comply with requirements of the Food and Drug Administration for information in the published literature about submitted and related drugs for inclusion in IND and NDA documents.

Retrieval from the ABLS is by means of bibliographies or by lists of descriptors together with accession numbers. Lists of descriptors with accession numbers and microfilm of all articles in the system are a particularly useful tool for rapid answering of questions. Bibliographies may be printed both with or without descriptors. Retrieval may be made on single or multiple terms. At present, there are approximately 16,000 condensates and about 8,600 descriptors in the ABLS. Condensates are entered currently at an annual rate of about 4,900; about 800 new descriptors are added each year.

Knowledge of articles for input to the ABLS is obtained by inspection of primary journals and the secondary sources ASCA, DRUGDOC, MEDLARS, Biological Abstracts, Bioresearch Index, Drugs in Prospect, Drugs in Research, and Drugs in Use.

Information about pharmaceutical patents of interest is distributed in a bulletin, Current Medicinal Patents, derived from the FARMDOC portion of Central Patents Index.

Our most recent current awareness system, introduced in January 1973, involves current chemical market information and is obtained from Predicasts' Current Market Abstracts tape. In cooperation with the ICI United States Management Information Services Department, a computer system was devised to enable preparation of bulletins containing abstracts from this tape service. These abstracts are disseminated in five monthly bulletins covering different subject areas (Figure 3). Although the current chemical market abstracts bulletins are available to members of the various research and development departments, they are aimed principally at marketing and marketing research personnel. Subjects covered are related to the present line of ICI United States products. Initially a part of our computer system for handling the Predicasts CMA tape included a capability for cumulating the tapes and performing retrospective searches. With the advent of the on-line system PATS in 1974, derived from the same data base, we have shifted to this more efficient system for retrospective searches of chemical market and business information.

INTERNAL RESEARCH DATA

Internal chemical and preclinical research data are recorded in two separate but related computer systems.

KWOC LIST OF COMPOUND NAMES AND COMPOUND NUMBERS

GLYCOL

PROPYLENE GLYCOL MONO-STEARATE	G-2180
ALDO 25 ...PROPYLENE GLYCOL STEARATE	X11100012
PLURONIC L44 ...POLY-OXYETHYLENE-OXYPROPYLENE GLYCOL	X11102017
PROPYLENE GLYCOL	Z03080022

STEARATE

PROPYLENE GLYCOL MONO-STEARATE	G-2180
ALDO 25 ...PROPYLENE GLYCOL STEARATE	X11100012

Figure 4. Portions of KWOC list of compound names and compound numbers illustrating multiple citation of names with glycol and stearate.

The chemical research system, which was described earlier,[5] provides for multiple types of data pertaining to each research or reference compound. Data can be recorded for each compound on its identity, constitutive properties, analytical data, physical properties, and results of tests of utility. Entry to the computer is by punched cards. Each card holds specific data, a card code identifying the type of data, and a compound number. There are approximately 300 different card types in the system, each representing a different characteristic, property, or test of utility.

Initially the IBM 870 Document Writer was used for both input and output. Presently the Document Writer is used chiefly to prepare proof copies of information on punched cards. Most printouts now are obtained from our IBM 370/145 computer.

Output can include printouts of information concerning specific compounds or of all compounds for which specific properties or use test results have been determined. Besides the molecular formula used for all compounds in the system, a fragmentation code containing approximately 200 fragments is used to describe the constitution of nondrug candidates and reference compounds. Information in the names of compounds can be used advantageously to select compounds and classes of interest.[6] Thus KWOC lists are prepared which consist of fragments of names together with compound numbers. Portions of such a list are illustrated in Figure 4, showing multiple listing of some glycol and stearate compounds. Although fine structural discrimination cannot be achieved by use of such KWOC lists, any group which forms part of a chemical name (*e.g.*, trifluoromethyl, sulfonyl) can be retrieved easily.

Biomedical Research data are recorded in a parallel system which contains the results of 26 pharmacology and three toxicology tests. Retrieval may be made by type of test, test result, or class of compounds. The constitution of drug candidates and drug reference compounds are recorded in Wiswesser Line Notation rather than the fragmentation code, because of the much greater amount of information which it contains.

To recapitulate, the Research Information Section supports the development and prosecution of the ICI United States research program and supplies information to nonresearch units by collecting, evaluating, and summarizing relevant scientific and technical publications, by selecting and disseminating current literature, and by recording and retrieving internal research data.

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ences; TOXLINE, National Library of Medicine, toxicologic abstracts and references; CHEMCON, Chemical Abstracts Service, chemical references; PATS, Predicasts Inc., chemical marketing abstracts and references.

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The Hercules Technical Information Division: Services, Special Systems, and R&D†

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The following information groups and services in the Hercules Technical Information Division are described: Library (open literature); Files (Hercules proprietary literature); Translating; Editorial; Report, Journal, and Patent Literature; Literature Research; Chemical and Market Data; Computer and Mathematics; and Computerized Information Systems Design and Programming. Several special information systems and the place of R&D in the various operations and services are discussed.

Five years ago, I presented a paper[10] on "Management of Operations and Services in the Hercules Technical Information Division" at the 4th Middle Atlantic Regional Meeting, February, 1969. Two points I directed attention to in that paper were: the need to change technical information operations and services in harmony with changes in objectives and goals of the parent organization; and the need to design new operations and services to meet new needs.

Many changes have occurred over the past five years, not only in chemistry and chemical technology, but also in the organizational set-up of Hercules, the Research Center, and the Technical Information Division. The charts I used five years ago to illustrate the organizational set-up of the Research Center and of the Technical Information Division are now a part of our history. The current organizational set-up of the Research Center is shown in Figure 1 and that of the Technical Information Division in Figure 2.

Obtaining, storing, and circulating documents are basic to all information operations.[2,8] There are, however, three primary categories of documents which are essential components in information services within an industrial R&D environment:

1. Documents generally housed in a library, such as books, journals, patents, trade publications, and available to everyone for purchase.
2. Technical reports, generally housed in a special Report Files, written by or for R&D personnel and relevant to the ongoing R&D programs.
3. Technical correspondence, generally housed in a Correspondence Files, which, in a sense, is supplementary to and complements the Report Files.

Both the Report Files and Correspondence Files are unique for Hercules; they exist to protect proprietary information but within a system that makes the documents readily accessible to those with a need to know.

These three document services, Library, Report Files, and Correspondence Files, constitute our information problem when viewed in terms of size, growth, and complexity. They also constitute an important and essential raw material base on which we can build new science and new technology, and by which scientists and engineers can know what is known in all areas of interests pertinent to the company's business and future growth.

LIBRARY

The Hercules Research Center Library contains over 30,000 books and bound volumes of journals, thousands of U. S. and foreign patents, all trade publications of interest to the needs of R&D personnel for chemicals and equipment, and other documents, and subscribes to approximately 700 journals. One of the objectives of the Library is to have books on the shelves before someone from the laboratories asks for them. Because the head librarian maintains a constant awareness of our R&D programs and of who is doing what, he is unusually successful in anticipating our needs for new books and in keeping journal subscriptions in harmony with our scientific and technological interests.

An extremely important service of the library is the circulation of journals routinely to those who need them on a continuing basis. So that the library can have journals available in the library during the working day and still serve readers routinely, the library subscribes to as many copies as necessary to accomplish both and to handle requests for specific articles. Routine journal circulation is handled by a computer system which matches each copy of a requested journal with the requesters by building number and room number on a computer-produced circulation card. The computer system is also tied in with the library's subscription order.

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