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INFORMATION RETRIEVAL IN TOXICOLOGY[1]

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INTRODUCTION

In preparing this chapter, it was important first to identify the probable audience of readers, and second to select those information activities, systems, projects, and trends that would be of particular interest and value to these readers. Based on the content of previous volumes, one assumes that the main readership of the *Annual Review of Pharmacology and Toxicology* consists of research scientists who utilize scientific and technical information in pursuit of their scientific endeavors. Consequently, descriptions of only those developments in the scientific and technical information field that would be of interest to these "end users," i.e. the practitioners in toxicology, pharmacology, and allied sciences, have been emphasized.

This chapter, which has been structured according to the sequential stages in the communications structure of science (1), identifies primary, secondary, and tertiary publications and services, and describes certain information storage and delivery systems. Emphasis is placed on delineating online information retrieval systems, since it is in this area that the most rapid developments, holding the greatest promise for the information user, are taking place.

Toxicological Information

In its 1966 report on the handling of toxicological information (hereinafter referred to as the PSAC Report), a panel of the President's Science Advisory Committee defined toxicological information as "all information de-

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scriptive of the effects of chemicals on living organisms or their component subsystems" (2). The "effects of chemicals on living organisms" is an area of growing scientific and public concern.

In the 13 years since the issuance of this report, this concern has manifested itself in new chemical regulatory legislation such as the Toxic Substances Control Act, the Occupational Safety and Health Act, and others. Indeed, chemicals are now regulated under 15 major US laws (3). During this period, we have also seen the birth of new government agencies such as the Environmental Protection Agency, the Consumer Product Safety Commission, and the Occupational Safety and Health Administration, whose principal mission is the regulation and control of chemicals. Substantial new governmental research efforts concerning the health and environmental effects of chemicals have become a major focus of the National Cancer Institute, the National Institute for Environmental Health Sciences, and the National Institute for Occupational Safety and Health. There has been an accompanying increase in toxicology testing and research in the chemical and pharmaceutical industries.

The PSAC Report stated that toxicological information "is generated in every part of the globe, is published in many languages and finds its way into the basic bibliographic network through a multiplicity of channels. The system for accomplishing this dissemination is vast, complex, and varies considerably in its sophistication" (4). As any user of toxicological information knows, this picture is still accurate. In fact, the volume of published toxicological information is increasing faster than any other segment of the literature. Baker (5) reported that the toxicology section of *Chemical Abstracts* increased by 345% between 1971–1975, while all of *Chemical Abstracts* grew by only 41.8%. Attempts to simplify, expand, and improve access to toxicological information are under way, mostly through the increased application of computers and communications systems for information storage, processing, and retrieval.

Among the recommendations proposed in the PSAC Report was the development of "a computer-based system for handling toxicological information ... within HEW" (6). In 1967, this recommendation was implemented through the establishment of the Toxicology Information Program in the National Library of Medicine (7).

PRIMARY PUBLICATIONS

A primary publication has been defined as "one that first records the results of R&D in the literature for broad distribution and use by the entire science community" (L. Bernstein and E. Siegel, unpublished report).

Primary Journals

Toxicological information is dispersed over a broad set of primary journals. The PSAC Report (2) estimates that the body of primary publications relevant to toxicology includes 1066 journals. More recently Ross (8) listed some 1100 periodicals important to the "toxic substances" area.

Surprisingly, a search of the journal citations carried in the online, bibliographic retrieval service TOXLINE (see below) indicates a much greater dispersion. Over 14,500 journals are cited at least once. The 100 most frequently cited journals are listed in Table 1. However, as expected, these 100 (i.e. 0.68% of the set of 14,500) are responsible for 29% of the journal articles in TOXLINE (F. Bayard, unpublished results).

Report Literature

A full discussion of the scientific and technical report literature—another segment of the published literature—is beyond the scope of this review. Suffice it to say that reports which often contain primary information are a medium heavily used by US Government agencies and their contractors. An analysis of 1965–1975 (with estimates to 1980) report distribution figures is given by King (9). Most US Government reports are published by, or made available through, the National Technical Information Service (NTIS) (10) and the Government Printing Office (GPO) (11). The major announcement journal for NTIS is the biweekly *Government Reports Announcements and Index* (10), which describes some 70,000 new technical summaries and reports annually. Most of these can be obtained on microfiche directly from NTIS. Standing order microfiche services called *Selected Research in Microfiche* (SRIM) are available in selected subject areas. Abstract newsletters are produced in 26 subject areas including agriculture and food, environmental pollution and control, and medicine and biology. Both SRIM and the newsletters are available by subscription from NTIS (10).

An NTIS Bibliographic Data File is available for online searching from three commercial services, BRS (12), Lockheed (13), and SDC (14), and comparisons of the results of searching this file in different systems have been reported (15, 16). The *GPO Monthly Catalogue of United States Government Publications* (17) is available through subscription or may be searched online through Lockheed.

The Department of Health, Education, and Welfare Committee to Coordinate Environmental and Related Programs (DHEW CCERP) (formerly DHEW Committee to Coordinate Toxicology and Related Programs) is sponsoring a project called Toxicology Document and Data Depository (TD3) (18) which has as its goals (*a*) identification of toxicology-related

Table 1 Primary journals with toxicological information

Acta Pharmacol. Toxicol.	*IRCS Med. Sci.*
Am. Ind. Hyg. Assoc. J.	*Indian J. Exp. Biol.*
Am. J. Obstet. Gynecol.	*Jpn. J. Pharmacol.*
Am. J. Physiol.	*J. Agric. Food Chem.*
Am. Rev. Respir. Dis.	*J. Air Pollut. Control Assoc.*
Anal. Chem.	*J. Am. Med. Assoc.*
Anesthesiology	*J. Assoc. Off. Anal. Chem.*
Ann. Intern. Med.	*J. Bacteriol.*
Ann. NY Acad. Sci.	*J. Biol. Chem.*
Antibiotiki	*J. Chromatogr.*
Antimicrob. Agents Chemother.	*J. Dent. Res.*
Arch. Environ. Health	*J. Econ. Entomol.*
Arch. Int. Pharmacodyn. Ther.	*J. Endocrinol.*
Arzneim. Forsch.	*J. Med. Chem.*
Atmos. Environ.	*J. Natl. Cancer Inst.*
Biochem. Biophy. Res. Commun.	*J. Pharm. Sci.*
Biochem. J.	*J. Pharmacol. Exp. Ther.*
Biochem. Pharmacol.	*J. Pharm. Pharmacol.*
Biochim. Biophys. Acta	*J. Physiol.*
Biull. Eksp. Biol. Med.	*J. Toxicol. Environ. Health*
Brain Res.	*J. Water Pollut. Control Fed.*
Br. J. Cancer	*Khim-Farm. Zh.*
Br. J. Pharmacol.	*Lancet*
Br. Med. J.	*Life Sci.*
Bull. Environ. Contam. Toxicol.	*Med. J. Aust.*
Cancer	*Mutat. Res.*
Cancer Res.	*Nature*
Chem. Pharm. Bull.	*Nauch. Tr. Novsib. Med. Inst.*
Chem. Biol. Interact.	*Naunyn Schmeidebergs Arch. Pharmacol.*
Clin. Pharmacol. Ther.	*Neuropharmacology*
C. R. Acad. Sci.	*N. Engl. J. Med.*
C. R. Soc. Biol.	*Nouv. Presse Med.*
Dtsch. Med. Wochenschr.	*Oyo Yakuri*
Endocrinology	*Pharmacol.*
Environ. Health Perspect.	*Pharmazie*
Environ. Res.	*Poult. Sci.*
Environ. Sci. Tech.	*Proc. Natl. Acad. Sci. USA*
Eur. J. Pharmacol.	*Proc. Soc. Exp. Biol. Med.*
Experientia	*Prostaglandins*
Exp. Cell. Res.	*Radiat. Res.*
Farmakol. Toksikol.	*Radiobiologiia*
Farmatsiya Resp. Mezhved. Sb.	*Res. Commun. Chem. Pathol. Pharmacol.*
Febs. Lett.	*Science*
Fed. Proc.	*Teratology*
Food Cosmet. Toxicol.	*Toxicology*
Gastroenterology	*Toxicol. Appl. Pharmacol.*
Genetics	*Toxicon*
Genetika	*Vopr. Onkol.*
Gig. Sanit.	*Water Res.*
Gig. Tr. Prof. Zabol.	
Health Phys.	

documents within the NTIS system, (*b*) enrichment of NTIS with toxicology-related documents (mostly agency reports) that now are not submitted to that organization, (*c*) announcement of toxicology-related NTIS documents in the online retrieval system TOXLINE, and (*d*) inexpensive dissemination of these documents in hard copy or microfiche from NTIS. Some portions of the TD3 project will become available in 1979. An analysis of four issues of the 1977 *Government Reports Announcement and Index* (10) for content germane to toxicology (F. Bayard, unpublished study) indicated that some 13% of the records (i.e. approximately 9000/year) could be so classified.

Scientific Meetings

The functions of the scientific meeting in the communication of science were analyzed by Lin, Garvey & Nelson (1). Various aspects of toxicology and pharmacoloy are represented at a variety of national and international meetings and specialized conferences. A list of some 96 conferences, from 1975 through 1977, concerned with toxic substances was assembled by Ross (19).

Published meeting proceedings have increased by 40% in the period 1965–1971 (9). While some proceedings are referenced by the major secondary systems such as *Chemical Abstracts* and *Biological Abstracts,* retrieval of information presented at meetings is usually not easy. Two new journals, the monthly *Index to Scientific and Technical Proceedings* (20) (indexing 90,000 papers from 3000 proceedings per year) and *Conference Papers Index* (referring in toto to 530,000 papers from 5000 conferences) cover the content of meetings, conferences, and symposia. *Conference Papers Index* also will be available for online searching through Lockheed and SDC (21, 22).

COMPUTER CONFERENCING Computer conferencing is a new, computer-mediated form of interaction among "geographically dispersed groups of people who must regularly exchange information and opinions" (23). Participants communicate via their computer terminals, using a central computer as their message center. Experiments in this area have been pioneered through a National Science Foundation–sponsored Electronic Information Exchange System. Hiltz & Turoff describe the topic and its implication for science communication in their recent book, *The Network Nation* (24). The authors do not report on any formal computer conferencing experiments in toxicology.

PROPHET, an older online system used for biological data handling, has some aspects of computer conferencing (25). It should be noted that most online, interactive retrieval systems (see below) lend themselves, theoretically, to the communications required for this technique. Therefore it is likely that, in the future, some of the online retrieval systems containing toxicological information will be used for such direct communications among users.

SECONDARY INFORMATION SERVICES

Secondary information services, also referred to as bibliographic abstracting and indexing or A & I services: "acquire . . . books, journal articles, patents, dissertations, technical reports, etc.; analyze these documents; usually provide a bibliographic description of each document; index each document according to a predetermined subject analysis system; and, periodically, produce a product which provides subject access to the references to all documents covered by the service during that time period" (26). A & I services function predominantly as "fact locators" rather than "fact providers." In other words, they direct the searcher to a document that contains the looked-for fact or datum, rather than providing him with the fact itself, in the sense that a handbook of tables does. Worldwide, some 2500 secondary services are available in all subject areas (27). Of these, over 300 are computer-readable, many of them providing the content of the online, interactive retrieval systems now widely available (see below).

Two major A & I services relevant to toxicology have been reviewed during the last four years, namely, *Chemical Abstracts* by Baker (5) and by O'Dette (28), and *Biological Abstracts* by Steere (29).

Another approach to processing the primary literature into a secondary retrieval system consists of listing the references cited in a given article instead of abstracting its subject content. The information service based on this concept is made available in printed form as the *Science Citation Index* (30) and as an online, interactive retrieval file, called SCISEARCH, from Lockheed (22). The principles of citation indexing have been reviewed by Weinstock in 1971 (31) and quite recently by Garfield (32).

While the major secondary services, mentioned above, include subject areas pertinent to toxicology, the literature in this field is also covered by a series of specialized, secondary publications. Gillespie (33) and Madden & MacDonald (34) review drug information sources; poison control information resources are described by Veltri & Temple (35); and cosmetic information sources are described by Johnson & Radar (36).

In addition to providing users with the means to locate older literature, many secondary information services also play an important role in current awareness, that is, in keeping users informed about new developments in their fields. Several of the major secondary services publish "spin-off" current awareness publications; some of these pertain to toxicology. For example, the relatively new series, *CA Selects* (37), from Chemical Abstracts Service (CAS) includes among its 80 titles the following: *Carcinogens, Mutagens and Teratogens; Chemical Hazards; Health and Safety; Drug and Cosmetic Toxicity; Food Toxicity;* and *Forensic Chemistry.*

BioSciences Information Service (BIOSIS) (38) produces two current awareness series from *Biological Abstracts:* (*a*) *Bioresearch Today* (14 topics) including topics such as *Birth Defects, Cancerogenesis,* and *Industrial Health and Toxicology,* and (*b*) *BIOSIS Standard Profiles* (28 research topics) with profiles on *Developmental Defects—Drugs, Pesticide Residues in Foods,* and *Monitoring of Environmental Pollution.* BIOSIS also publishes *Abstracts of Health Effects of Environmental Pollutants,* with approximately 1000 references per month.

From the *Science Citation Index* (30) data base, the Institute for Scientific Information furnishes a weekly service called ASCA (Automatic Subject Citation Alert) wherein a user can request to be kept aware of all papers citing a given "lead" paper, author, or subject area. A related service, ASCATOPICS, reports on standard interest profiles.

In order to support their basic missions, the major secondary services often have to maintain ancillary operations and functions. For example, BIOSIS maintains a taxonomic system, BioSystematic Codes (29); the National Library of Medicine keeps up a controlled vocabulary system called MeSH (Medical Subject Headings) (39); and CAS maintains a computerized registry system for chemical compounds (40–43). In this CAS Registry System, every compound newly described in the primary literature covered by *Chemical Abstracts* is given a unique CAS Registry Number, through which it is possible to access structural, nomenclature, and other information categories in the CAS computer system. The CAS Registry Number has become an important identification code for chemical compounds and is now carried in many computer files and printed sources, worldwide. The CAS Registry System contains information about some 4 million compounds.

TERTIARY PUBLICATIONS

"A tertiary publication is one in which the emphasis is on providing organized, broad, critical overviews of known (or "old") information, and in which presentation of new information is absent, or at best incidental" (L. Bernstein and E. Siegel, unpublished report). Books and many monographs are included in this category. This section of the review presents a short overview of where information about this category of publications can be found.

Obviously, good sources of information about new books are the book review sections of professional journals. In 1974, Chen & Wright (44) analyzed book reviewing in biomedicine and listed the ten top biomedical book–reviewing journals.

Information about new books and monographs is also provided by the major A & I services and, therefore, appears in some of the online, bibliographic retrieval services (e.g. TOXLINE). The National Library of Medicine (NLM) publishes the monthly *Current Catalog* (45) with information about recent books and serials in biomedicine. The *Current Catalog* is also available online as the CATLINE service from NLM (22). Other online cataloging services, while mainly "library tools," do provide subject access and, therefore, can be used to identify publications in particular subject areas. Several of these services have been reviewed recently by McCarn (46).

A number of US Government, international, academic, and industrial organizations produce monographic series of importance to toxicology. Examples are *Criteria for a Recommended Standard: Occupational Exposure to . . .* by the National Institute for Occupational Safety and Health, *Bioassay of . . . for Possible Carcinogenicity* by the National Cancer Institute, and *IARC MONOGRAPHS on the Evaluation of Carcinogenic Risk of Chemicals to Humans* by the International Agency for Research on Cancer.

Preparation of these monographic series frequently involves the work of committees of experts, often at great expense to their sponsoring organizations—usually government agencies. In order to prevent unknowing duplication of monograph preparation within government, the DHEW CCERP initiated a *Chemical Monograph Referral Center* (CHEMRiC) in collaboration with the Consumer Product Safety Commission. Agencies can report their monograph preparation plans to CHEMRiC and, conversely, learn from CHEMRiC about planned, ongoing, or completed monographs sponsored by other agencies (47).

In many cases, the announcement and dissemination of these monographs compare poorly with the much wider distribution, better reviewing, and more systematic archival storage given to commercially produced books, which most often are created for only a fraction of the resources applied to the preparation of the government-sponsored monographs.

STORAGE AND DELIVERY SYSTEMS

Online Retrieval Services

Online retrieval services have become widely available during the last 10 years. In accessing these services, the searcher uses a typewriter-like, computer terminal linked either directly or through a (usually) telephone-based communications network (48) to a computer in which the information is stored. General requirements for such services are computer-readable data bases; computers with massive, random access storage devices (hardware); search programs (software); communications networks and user terminals (hardware). Online retrieval services have recently been reviewed by McCarn (46) and Hall (49). Hawkins (50) provides a useful bibliography of the literature concerning these services.

Online information retrieval systems can be divided into bibliographic and data retrieval systems. The former provide references to the location of data in the primary literature, reports, or monographs. The latter deliver the actual data sought by the searcher (51).

In 1978 there were 55 million bibliographic references available online (52), up from 33 million in 1976 (53). From 1974 to 1977, the number of online searches grew from 700,000 to over 2,000,000 annually (53). Increased availability of online services is due to a long-term trend of decreasing computer costs including storage (49) and better, less expensive communications. The growing popularity of online retrieval can be attributed to its offering the possibility of (*a*) rapid and relatively inexpensive searching of voluminous data bases and (*b*) interaction by the searcher with the system, permitting examination of a sample of the output, and alteration of the search strategy if that sample is not satisfactory.

In the United States, online services are made available by several major information suppliers including Bibliographic Retrieval Service (BRS) (12), Lockheed Information Service (Lockheed) (13), National Library of Medicine (NLM), (54–56) and the System Development Corporation (SDC) (14).

The major online services vendors use different software and require different access and search routines. Each also provides its users access to a collection of different data bases. On the other hand, the same data base may be available from several suppliers, often at different costs, and frequently requiring different search strategies and procedures (46). It is not surprising that this Balkan-like scenario confuses the scientist/end user and, in many cases, keeps him from using online systems directly (52). Instead, there are professionals—information intermediaries—who function as agents for the end user and search the various systems and data bases as required. While this type of arrangement may contribute to efficient use of these systems, it also reduces the potential power of online searching by removing the end user from real interaction with the systems (46).

Sewell & Bevan (57) have shown that involvement of the scientist/user (pathologists, pharmacists) in online searching improves utility of the product. Jahoda & Bayer (58) compared the effectiveness of mediated and unmediated online searching by industrial and academic scientists, and Meadows (59) predicts increasing use of online retrieval systems by end users. Williams points out that systems "friendly" to end users not only will be used more effectively but will also be cheaper "by virtue of eliminating (in most cases) the necessity for an intermediary searcher between the end user and the system" (60).

The growing use of online, bibliographic retrieval services has increased demand for copies of the original articles cited in the data bases. Some online service providers allow the user to order copies of required documents online (61). In general, however, the expansion in demand for article copies has placed an added burden on the interlibrary loan services of libraries. These services are reviewed for research libraries in general (62), and for the Regional Medical Libraries in particular (63, 64).

The United States has led the world in the development of online information retrieval systems because of the earlier availability of the required computers and also because this country had a relatively uniform, nationwide, telephone-based communications system. However, other regions such as Canada, Western Europe, Japan, and Australia are rapidly increasing their use of online systems (65, 66). While US-generated online data bases are widely available outside this country, the reverse is, as yet, less true. Nevertheless, certain biomedical and environmental data bases (67, 49) developed in Western Europe are becoming available, online, in this country through US service providers. An up-to-date list of data bases available from six services in Europe and the United States was published in 1978 by *Online Review* (22).

BIBLIOGRAPHIC RETRIEVAL SERVICES IN TOXICOLOGY Information relevant to toxicology in its broadest sense can be found in many online, bibliographic retrieval systems. Among the 108 bibliographic data bases listed in a recent survey (67), some 33 can be classified as being relevant to this field. Bawden (68) provides a recent overview of online search services for "chemical toxicology."

By way of example, one such service, TOXLINE (Toxicological Information Online) is described here in greater detail. TOXLINE was created by NLM's Toxicology Information Program in 1974 to provide an online, interactive, bibliographic retrieval service specifically designed for toxicology. Since toxicology did not have a unified, indexed data base that could be offered online, it was necessary to develop such a file by amalgamating "toxicology subsets" of other, secondary services with relevance to biomedicine and the environment. Thus, TOXLINE now contains subsets (33, 69) from *Index Medicus, Chemical Abstracts,* and *Biological Abstracts* plus the following (in toto): *International Pharmaceutical Abstracts, Pesticide Abstracts,* and the bibliographic files of the Environmental Mutagen and Environmental Teratology Information Centers. Recently, a "toxicology" subset from the ongoing research information data base of the Smithsonian Science Information Exchange (70) was added to the file. TOXLINE's coverage and utility as compared to that of *Excerpta Medica* have been reported (69, 71).

In its architecture, TOXLINE represents a "tertiary data base" (72); that is, it has a special subject orientation and is synthesized or repackaged from several, relevant secondary services. The special management problems involving standardization of differently formatted records, proprietary and copyright interests, and other issues pertaining to tertiary data bases are described by Brandhorst & Williams (72).

TOXLINE now contains some 580,000 records (1974 to present) online, and 380,000 records for offline searching in a backfile called TOXBACK (1965–1973). In 1978 over 47,000 online searches were carried out in TOXLINE (73) and some 2 million citations and abstracts were provided to users, offline, through the mails. The service is available to over 900 organizations that have user agreements with NLM. Outside the United States, TOXLINE is provided through agreements with information dissemination organizations in Canada, France, Germany, Japan, Sweden, and the United Kingdom.

Free text searching, as employed in TOXLINE and in most other online, bibliographic services, uses essentially all words appearing in the title, abstract, and keyword fields of the records. This approach develops a large "vocabulary" in the computer (74, 75). Using free text searching relieves the user of the need to learn a standard vocabulary (e.g. MeSH in MEDLINE) (39) and thus may make online searching easier for the scientist/researcher actually requiring the information (57). However, in order to retrieve "complete" sets of records on a specific topic from a given file, the free text searcher must state his query in many different ways so as to incorporate the synonyms and alternative concept statements that might have been employed by the various sources in the file. This sort of exhaustive searching is made easier by controlled vocabulary indexing, for example, as it is used in MEDLINE.

Another online, bibliographic retrieval service of major importance for biomedicine, in general, is NLM's MEDLINE (MEDical Literature Analysis and Retrieval System on-LINE) service. With 460,000 online searches performed against the MEDLINE file in 1978 (73), MEDLINE is one of the most heavily used online, bibliographic retrieval services in the world (46). The service and the file have been described thoroughly in the literature (54–56). A 1978 issue of *Medical Informatics,* devoted entirely to MEDLINE, includes articles on training (76), usage (77), communications

(78), hardware and software (79), searching (80), online user network (64), and article selection, thesaurus building, and indexing (39). MEDLINE is also offered as a service by BRS (12).

Other toxicologically relevant, online, bibliographic services now available are AGRICOLA (agricultural information), *Biological Abstracts, Chemical Abstracts,* CANCERLIT, ENVIROLINE, EPILEPSYLINE, *Excerpta Medica, Food Science and Technology Abstracts,* PESTDOC (pesticide literature), *Pollution Abstracts,* and RINGDOC (pharmaceutical literature) (67, 22). A somewhat different list of online services, seen from a European perspective, is provided by Hall (49).

RETRIEVAL SERVICES FOR CHEMICAL INFORMATION Inasmuch as toxicology deals predominantly with the effects of chemical substances on biological systems, the handling of chemical information is an important area of toxicology information retrieval. TOXLINE, for example, carries CAS Registry Numbers as searchable entities. TOXLINE is also backed up by an online "chemical dictionary," CHEMLINE (81, 82), which can be searched online using standardized *Chemical Abstracts* nomenclature, synonyms, molecular formulae, CAS Registry Numbers, and ring structure data. CHEMLINE, essentially a subset of the CAS Registry System (40–42), is organized by compound, and specifically contains records for some 400,000 compounds mentioned in TOXLINE, TOXBACK, and in certain other files. Through an online, searchable "locator" field CHEMLINE refers the user to other data bases such as TOXLINE, TOXBACK, Toxicology Data Bank (TDB), Registry of Toxic Effects of Chemical Substances (RTECS), Toxic Substances Control Act Inventory, and the New Drug Application (NDA) files of the Food and Drug Administration. CHEMLINE also provides substructure search capabilities, insofar as fragments of molecular formulae, standardized nomenclature, and certain ring information fields are searchable (82, 83).

Online, chemical information files, similar to CHEMLINE in organization and content, and fulfilling analogous functions, are also provided by SDC (14) as CHEMDEX and by Lockheed (13) as CHEMNAME (84). A somewhat differently structured online, chemical search service is offered by the Chemical Information System (CIS) (85–87).

DATA RETRIEVAL SERVICES IN TOXICOLOGY In the context of this review "data" can be verbal (i.e. a statement describing a fact or datum) or numeric. It is also useful to separate data bases into those that contain only published data and those that are composed of unpublished data (e.g. laboratory measurements). Usage and validation aspects applying to data bases fitting into these categories have been discussed (51).

Luedke (88) estimates that in 1977 there were 150–300 numeric data base systems available for online access in the United States and 200–400 worldwide. The European Association of Scientific Information Dissemination Centers (EUSIDIC) published an international list of 246 nonbibliographic data bases (89).

Tomberg (65) believes that, worldwide, the growth of online data banks will outstrip that of the bibliographic systems. A detailed review of numeric data bases, including online services, has been published recently (90).

Only a few of the publicly available online data retrieval systems are germane to toxicology. Bracken et al (91) have described a variety of such systems (mostly government-sponsored) that are relevant to various aspects of the Toxic Substances Control Act.

The NLM offers two online data retrieval systems reporting published toxicological data: (*a*) RTECS (Registry of Toxic Effects of Chemical Substances) and (*b*) the Toxicology Data Bank. RTECS is the online version of the annual National Institute for Occupational Safety and Health publication by the same name (92) (formerly the *Toxic Substances List*). It contains acute toxicity values for some 36,000 substances; some carcinogenicity and aquatic toxicity data are also available. Online, coordinate searching by substance name, test animal, and route of administration is possible and references to published sources of the data are provided. The online file is updated quarterly (93).

The Toxicology Data Bank (TDB) (94, 95) describes the chemical, physical, biological, and usage attributes of toxic or potentially toxic chemicals to which populations are exposed. Data in over 60 subject categories are extracted from some 80 evaluated, published sources (e.g. textbooks, handbooks) and are further evaluated by a committee of experts (96). TDB now contains some 1200 compound records (97) and grows by approximately 150 records quarterly. RTECS and TDB are both linked to CHEMLINE through the CAS Registry Numbers of the compounds they describe. Thus, the online user can perform substructure or nomenclature searches in CHEMLINE and then find related biological data in the other files.

The National Institutes of Health and the Environmental Protection Agency sponsor the Chemical Information System (CIS) which provides online, interactive access to various physical data files, linked to a chemical structure search system. CIS includes mass spectra, carbon-13 nuclear magnetic resonance, X-ray crystal data, and X-ray powder diffraction data files as well as a variety of software modules for interactive searching of these and other data files (85–87).

The Laboratory Animal Data Bank (LADB), an online data retrieval system for animal data, is in the developmental stages and will be offered for public, online access in 1980. It contains hematology, clinical chemistry, pathology, and growth data for laboratory control animals, as well as environmental, husbandry, and nutrition data describing the conditions under which the animal groups are kept. Online statistical manipulation as well as data retrieval are possible. The system requires a minimum of training and has been designed for use by the laboratory scientist rather than by an information intermediary. Data for LADB do not come from the published literature but are provided voluntarily by participating industrial and governmental laboratories (51). At this writing (Spring 1979), LADB contains 314,000 observations on 25,700 animals, 29 species/strains (rodents, dogs, primates) in 180 groups from over 35 laboratories. Only short descriptions of this DHEW CCERP-sponsored project have been published (18, 98, 99).

INFORMATION CENTERS The role of the intermediary in online information retrieval has been mentioned (46). This function can be located in an information support facility such as a library in the researcher's organization. There are also "information broker" organizations performing literature searches on a fee-for-service basis for requestors. In some instances, such organizations specialize in particular subject areas. In biomedicine, for example, online literature searches are carried out by the 11 Regional Medical Libraries and many of the member institutions of NLM's online network (64). The NLM-supported Toxicology Information Response Center at the Oak Ridge National Laboratory (100, 101) is an information service that functions as an information center in toxicology. As described by Gerstner, Huff & Ulrickson (102), the center performs literature searches on demand, prepares annotated bibliographies, some with overviews, and publishes bibliographies on toxic chemicals (e.g. mirex, trichloroethylene, methoxyflurane) that are sold through the NTIS (10).

Ongoing Research Information

As the name indicates, ongoing research information (ORI) is concerned with information about research-in-progress or research-in-planning. In a recent review of ORI, Hersey (70) states that the collection, processing, and dissemination of ORI is needed to (*a*) avoid unwarranted duplication of research, (*b*) maximize utilization of R & D resources, and (*c*) coordinate planning of future R & D. ORI differs from "normal" bibliographic information in that (*a*) it is more difficult to obtain, (*b*) it has a definite shelf life, since publication of completed research results normally obviates the need for the earlier ORI record, and (*c*) the ORI record is usually the only available description of a given project; there is, as yet, no published paper.

A worldwide inventory of ORI services, called *Information Services on Research in Progress* (103), has been compiled. It lists 19 such services in the United States. The major US service for ORI as performed or sponsored by the government is the Smithsonian Science Information Exchange (SSIE) (70), which collects and processes ORI in a computerized data bank, from which it then provides various services. The SSIE data bank can be searched, online, through Lockheed and SDC (67).

A "toxicology" subset of the SSIE data bank is being identified and published monthly with approximately 1000 project descriptions as the *Toxicology Research Projects Directory* (104, 105). This publication is sponsored by the DHEW CCERP (18). Recently, the scope of this project was augmented by including epidemiology-related projects in the subset extracted from the SSIE data bank. The epidemiology portion will be published early in 1980 as an annual *Epidemiology Research Projects Directory* with approximately 3500 project descriptions. The abstracts from both publication sets are included, monthly, in the online retrieval service, TOXLINE (see above).

Information about ongoing or planned biological testing of chemicals also can be considered ORI. The need to avoid unknowing duplication of work is particularly important in this area in view of the great and increasing expense of such testing. Reports by industry and government agencies of planned or ongoing, long-term tests of compounds in animals, and epidemiological studies involving chemicals, are published monthly in *TOX-TIPS* (Toxicity Testing in Progress), another publication of the aforementioned DHEW CCERP (18, 104, 106).

Two other services providing ORI online are relevant to this discussion. The Current Research Information System (CRIS) (107) data bank, containing ORI from the US Department of Agriculture, is accessible online through Lockheed (22). The International Cancer Research Data Bank program of the National Cancer Institute collects ORI in the cancer field (108) from the SSIE data bank and from other, primarily international, sources. The information is made avilable online by the NLM as CANCERPROJ.

Networks

Online, interactive searching of large data bases represents a major advance in information retrieval. However, as has been described, the existing environment of multiple data bases dispersed in many computers and software systems, makes such retrieval complex and even clumsy, particularly for the occasional user. Often, an answer to a query necessitates the use of more than one data base (109, 110). In the best of circumstances, the required data bases are stored in one computer and the search system has been designed to facilitate coordinated, cross-data base searching (87). More often, however, searching must be sequential, with coordination of the information done external to the online search. Technical developments now make the construction of "systems of online systems," or networks possible. The term network, in this context, may be confusing, because reference has already been made to communications networks that are used to access computers from remote terminals (48). The networks under discussion here are systems of linked, "distributed (over several computers) data bases" (52). At one level, linkage can be accomplished by building logical interconnections, such as commonly held data elements, among data bases (52). This approach has been explored by Williams, who studied the feasibility of "mapping" among chemical data bases (111).

CHEMICAL SUBSTANCES INFORMATION NETWORK Another network project, in which linkage of online files will be brought about through computers and software, is the Chemical Substances Information Network now being implemented by a consortium of federal agencies. Since this project is particularly germane to toxicology, it is described here in greater detail.

In a study responding to requirements of Section 25b of the Toxic Substances Control Act of 1976 (112), Bracken et al (91) looked at (*a*) user needs for information arising from implementation of this new law, (*b*) available online and conventional information resources, and (*c*) requirements for new data bases.

They recommended that function-specific data bases, often residing in different government or private sector computers, containing information about toxicology, epidemiology, chemical and physical properties, manufacturing methods, product usage, laws and regulations governing the manufacture and use of chemical products, testing data, and other categories, should be included in an integrated, online Chemical Substance Information Network (CSIN).

Two online directory files, a Chemical Data Bases Directory and a Chemical Structure and Nomenclature System, will be constructed; they will point users to whichever files in the network contain the desired information about a compound or a group of chemically related compounds. As the technical capabilities of the system grow, it will perform increasingly more complex activities for the user. Eventually, it will obtain required data in an integrated fashion from several relevant data bases located in different computers.

The CSIN project is being coordinated by the Interagency Toxic Substances Data Committee, chaired by the Environmental Protection Agency and the President's Council on Environmental Quality (113). CSIN is intended for use by federal agencies and the scientific community.

There is, at this time, a paucity of publications describing the CSIN project. The most recent descriptions are in a contractor's report (114) and in a conference paper (115). However, since the project promises to have a major impact on information retrieval in toxicology and related fields, it seemed timely to describe its beginnings in this review so that interested readers can watch the literature for further developments.

INTERNATIONAL NETWORK PROJECTS Substantial international efforts to build networks for online data and bibliographic information retrieval also are under way, especially in Europe. Detailed descriptions of these activities are beyond the scope of this review. Readers should be particularly aware of the Commission of the European Communities project, EURONET, which is both a communications network and a network of data bases, including major biomedical data bases. Reviews by Stern (116) and Tomberg (66) are relevant to this topic.

SUMMARY AND CONCLUSION

This chapter has attempted to show that information about the effects of chemicals on living systems is of increasing scientific and social concern. This kind of information is dispersed over many primary, secondary, and tertiary information sources. As is true for other areas of science and technology, information retrieval in toxicology is becoming increasingly computer-dependent. The advent of online, interactive information retrieval systems has been particularly important. This development has had desirable as well as some undesirable consequences. On the one hand, these online systems make the retrieval process faster and more accurate and exhaustive. On the other hand, the complexity of the search process and the disjointedness of the available systems tend to discourage information requestors/users from direct use of these systems. This has led to the interjection of the online information specialist into the retrieval process. However, technical developments indicate that this picture is changing and that more user-friendly systems are in the offing. Finally, one can also see that the next major development in this field is the network of subject-specific, online information retrieval and processing systems. One such network, the Chemical Substances Information Network, now in the "blueprint" stage, will be of particular importance to users of toxicological information.

In conclusion, it should be noted that "information" is not a trivial part of science and technology. The costs for scientific and technical information and communication in the United States, in 1975, are estimated at $10.9 billion or 28.8% of what was spent in that year on scientific and technical R & D activities (117). Clearly, the methods we use in managing scientific and technical information relate directy to how efficiently and effectively we manage science itself.

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