



Health effects of toxicants: Online knowledge support



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ABSTRACT

Research in toxicology generates vast quantities of data which reside on the Web and are subsequently appropriated and utilized to support further research. This data includes a broad spectrum of information about chemical, biological and radiological agents which can affect health, the nature of the effects, treatment, regulatory measures, and more. Information is structured in a variety of formats, including traditional databases, portals, prediction models, and decision making support tools. Online resources are created and housed by a variety of institutions, including libraries and government agencies. This paper focuses on three such institutions and the tools they offer to the public: the National Library of Medicine (NLM) and its Toxicology and Environmental Health Information Program, the United States Environmental Protection Agency (EPA), and the Organisation for Economic Co-operation and Development (OECD). Reference is also made to other relevant organizations.

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1. Introduction

Scientific research relies upon and contributes to an ever growing body of data and information, leading to subject specific knowledge frameworks which evolve over time. Historically, libraries have played a critical role as repositories of information (using the word in its broadest sense), and served as the primary access points for retrieval. Computerization, the advent of the Internet, and mobile devices have resulted in the digitization of virtually all forms of information, broken down geographic boundaries, and immeasurably aided in our ability to find whatever we are looking for, wherever we may be. Moreover, a vast amount of this is free. Some physical libraries have been at the forefront of innovating digital information tools but other organizations not traditionally in the business of information provision have also become adept at making large data sets available globally online at no cost to the user. The field of toxicology is just one scientific discipline that has benefited enormously from the electronic dissemination of

information. This paper will highlight electronic information available from three major suppliers of toxicity data – a US biomedical library, a US environmental regulatory agency, and a multi-lateral governmental forum headquartered in Europe, each of which has consolidated and linked various resources in portal-like products. It will also take a brief look at a handful of the many other worldwide online tools which can assist in the pursuit of toxicity data.

2. NLM and TEHIP

A component of the US National Institutes of Health (NIH), the National Library of Medicine (NLM), founded in 1836 and currently located in the Washington DC suburbs, is the world's largest biomedical library. Its Toxicology and Environmental Health Information Program (TEHIP) has been a leader and focal point for information related to health and other aspects of environmental toxicants since its inception in 1967 as the Toxicology Information Program. It was created in response to recommendations of the President's Science Advisory Committee (PSAC). The Committee's report (PSAC, 1966, Handling of Toxicological Information,

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Washington, DC, White House) concluded that “there exists an urgent need for a much more coordinated and more complete computer based file of toxicological information than any currently available and, further, that access to this file must be more generally available to all those legitimately needing such information.”

Today, nearly 50 years later, in first quarter of the 21st century, TEHIP continues to meet the needs of toxicologists and the public through state-of-the-art databases and other online tools. One can link to these resources through the Program's home page at sis.nlm.nih.gov/enviro.html. Most of its databases of relevance to environmental toxicants, and the subject of this paper, are accessible through its TOXNET (Toxicology Data Network) system at toxnet.nlm.nih.gov. TOXNET houses a cluster of databases covering an extensive array of information on potentially hazardous chemicals, and their health and environmental effects. It offers user-friendly searching and features such as relevancy ranking, flexible sorting, and downloading options. It is free online and publicly accessible worldwide. A number of TOXNET databases, briefly reviewed below, are also available for leasing.

2.1. ChemIDplus (<http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp>)

Chemical identification is often a key starting point to learning more about a chemical's properties and toxicity. TOXNET's ChemIDplus is a dictionary of over 400,000 chemicals. Chemical preferred names and synonyms, CAS Registry Numbers, molecular formulas and weights, and 3-D structures are included within the records. For any given chemical, there are many links to other NLM databases, to resources external to NLM (such as from the EPA, NIOSH, the OECD) and to federal and state regulatory lists on which the chemical might appear.

2.2. HSDB (Hazardous Substances Data Bank) (<http://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm>)

HSDB presents an across the board view of over 5600 potentially hazardous chemicals and their properties. While most often consulted for its substantial toxicity data, it is an excellent source for a myriad of other information, including:

- Human health effects
- Emergency medical treatment
- Animal toxicity studies
- Metabolism/pharmacokinetics
- Pharmacology
- Environmental fate & exposure
- Environmental standards & regulations
- Chemical/physical properties
- Chemical safety & handling
- Occupational exposure standards
- Manufacturing/use information
- Laboratory methods
- Special references
- Synonyms and identifiers
- Administrative information.

Each of the above broad categories of information is actually divided into more precise data fields. For example, the human health effects category contains the following fields: toxicity summary, evidence for carcinogenicity, human toxicity excerpts, skin, eye and respiratory irritations, drug warnings, medical surveillance, populations at special risk, probable routes of human exposure, body burden, average daily intake, reported fatal dose, and milk concentrations. Further classifications are also available for some fields. The study summaries presented within human toxicity excerpts, for instance, may be categorized by a variety of sub-fields such as human exposure studies, signs and symptoms, case reports, epidemiology studies, surveillance, biomonitoring, genotoxicity, alternative and in vitro tests and endocrine modulation.

Data in the non-human toxicity excerpts field is also classified by a number of sub-fields.

An NLM Chemical Selection Team is responsible for choosing chemicals for inclusion based upon factors such as degree of toxicity, level of exposure and production volume. Chemicals of interest to various US government agencies, regulatory and otherwise, as well as global organizations, are other sources used to locate candidate chemicals. Finally, chemicals which are newsworthy for a positive (e.g. the newest wonder drug) or negative (e.g. massive chemical spill) reason also receive priority consideration. Data are drawn from a core set of monographs, government documents, technical reports, and the primary journal literature. A distinguishing characteristic of HSDB is the peer-review process used to build it. Its Scientific Review Panel (SRP), a committee of 16 scientists with expertise cutting across the database's major subject areas, meets 3 times a year to review, add, edit, and update its chemical records, some 300 per meeting. Associated with each data statement in HSDB is one of three data quality tags, as follows:

- Peer reviewed – for data statements which have been peer reviewed by the SRP;
- QC reviewed – for data statements which have received a preliminary quality control review, but not yet been reviewed by the SRP;
- Unreviewed – for a limited number of data statements, such as industry submissions, which do not readily lend themselves to scientific review but which may contain useful information nonetheless.

HSDB continues to be enhanced with new information and features. In recent years, for example, there has been an increased effort made to include more data on radionuclides, nanoparticles, reptile, scorpion, and spider venoms, plant toxins, and antivenins. Newer generation pesticides are being included as are EPA “green” chemicals, and chemical warfare agents are being updated. Visual displays will accompany text where appropriate. These may include, for example, metabolic pathways, pictograms used in the Globally Harmonized System of Classification and Labeling of Chemicals (GHS), and graphics representing venomous or poisonous animals, and poisonous plants. An ecotoxicity data element has also been created with subheadings for birds and mammals, aquatic species, other terrestrial species, field studies, and accidental poisonings. Consumer summaries will be added to provide succinct and easy to understand information summarizing toxicity and other characteristics of HSDB chemicals.

2.3. TOXLINE (Toxicology Literature Online) (<http://toxnet.nlm.nih.gov/newtoxnet/toxline.htm>)

In library terminology, a bibliography is a list of works about a particular subject. These days, bibliographies include references to both printed and digital sources. TOXLINE is a bibliographic database containing citations to literature covering the biochemical, pharmacological, physiological, and toxicological effects of chemicals, including drugs. The majority of TOXLINE's citations include abstracts, indexing terms, and CAS (Chemical Abstracts Service) registry numbers. Updated weekly, TOXLINE's more than 4 million references date from as early as the 1840s to the present.

TOXLINE is derived from a number of sub-files, with the largest portion coming from NLM's PubMed/MEDLINE database. Complementing this is literature from the DART (Developmental and Reproductive Toxicology) database and technical reports from Federal Research in Progress (FEDRIP), Toxic Substances Control Act Test Submissions (TSCATS), Toxicology Document and Data Depository (NTIS), and Toxicology Research Projects (NIH Reporter). DART, funded by several agencies, is also searchable as a free-standing database of more than 200,000 journal references on teratology and other aspects of developmental and reproductive toxicology. Rounding out TOXLINE are 13 archival collections which, despite no longer being updated, still contain valuable references. Among these are the International Labor Office,

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