

To: John Zogorski, Bill Wilber
From: Patty Toccalino, Robyn Phillips, Julia Norman
Date: June 14, 2004
Subject: Progress Report #3 for Research Element #1: List of sources of physical-chemical property data and toxicity data for human and aquatic receptors (FY04)
cc: Jim Pankow

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Background – Contents of this Progress Report

This Progress Report a deliverable for Research Element #1 for FY04. Research Element #1 involves the development and evaluation of a strategy to prioritize compounds for inclusion in the NAWQA Program. A science-based strategy is being developed that can be used to rank order compounds and/or subgroups of compounds for human health via potential water consumption and for aquatic life. Because both the Human-Health Ranking Strategy (HHRS) and the Aquatic-Life Ranking Strategy (ALRS) will consider a variety of factors including environmental partitioning/modeling and toxicity data relevant to humans or aquatic life, it is necessary to identify available sources of physical-chemical property data and toxicity data.

This Progress Report lists and briefly describes the contents of (a) physical-chemical property data sources and (b) toxicity data sources for human and aquatic receptors that may be used in the development of the HHRS and ALRS. Physical-chemical and toxicity data are available from a number of governmental agencies, universities, non-profit organizations, and commercial sources; many of these data are readily available online.

Table 1. On-line sources of physical-chemical data.

[CASRN, Chemical Abstracts Registry Number; MW, molecular weight; BP, boiling point; MP, melting point; VP, vapor pressure; H, Henry's law constant; Koc, soil sorption coefficient; Kp, permeability constant; Kd, soil-water partition coefficient; Kow, octanol-water partition coefficient; pKa, dissociation constant; BCF, bioconcentration factor]

Title	Type of data provided	Reference
Agricultural Research Service (ARS) Database	CASRN, molecular formula, MW, physical state, BP, MP, decomposition point, heat of vaporization, hydrolysis and photolysis rate constants, VP, water solubility, organic solubility, H, log Kow, pKa, Kd, field dissipation, soil half life (aerobic, anaerobic).	(U.S. Department of Agriculture, 2001)
Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles	Registered trade names, synonyms, chemical formula and structure, MW, color, physical state, MP, BP, density, odor, water solubility, organic solubility, log Kow, log Koc, VP, H.	(Agency for Toxic Substances and Disease Registry, 2004a)
ASsessment Tools for the Evaluation of Risk (ASTER)	ASTER is an integration of the AQUIRE (table 4) toxic effects database and the QSAR system. The QSAR system includes a database of measured physicochemical properties such as MP, BP, VP, and water solubility. Due to security restrictions, ASTER is currently not publicly available. Technical support staff will conduct an ASTER search for persons affiliated with governmental offices.	(U. S. Environmental Protection Agency, 2004c)
BIODEG	Part of the Environmental Fate Database. Biodegradation data (data types not specified).	(National Information Services Corporation, 1996)
BIOLOG	Part of the Environmental Fate Database. Biodegradation data (data types not specified).	(National Information Services Corporation, 1998)
CHEMFATE	Part of the Environmental Fate Database. MP, BP, pKa, ultra violet absorption, Kow, water solubility, VP, H, evaporation from water, soil column transport, BCF, hydrolysis, oxidation, photolysis, microbial degradation.	(Syracuse Research Corporation, 2004a)
ChemFinder.Com	Density, refractive index, evaporation rate, flashpoint, MW, MP, BP, vapor density, VP, and water solubility, as well as references to other sources of physical-chemical data.	(Cambridge Soft, 2004)
Chemical Information System	Data from the databases DATALOG, ENVIROFATE, ISHOW, and SANSS, including MW, pKa, adsorption, BCF, biodegradation, H, hydrolysis, log Kow, photooxidation, ultraviolet absorption, volatilization, VP, water solubility, BP, MP, microbial degradation, oxidation, photolysis, Kd, soil column transport.	(National Information Services Corporation, 2003)
DATALOG	Part of the Environmental Fate Database. pKa, Koc, BCF, H, hydrolysis rate constant, Kow, VP, water solubility.	(Syracuse Research Corporation, 2004b)
ENVIROFATE	pKa, bioconcentration, BP, degradation in natural systems, H, hydrolysis, Kow, MP, oxidation, photolysis, soil absorption, soil column transport, soil monitoring, ultraviolet absorption, VP, volatilization, water solubility.	(National Information Services Corporation, 1990a)
Environmental Fate Database (demo)	Data from the commercial databases DATALOG, CHEMFATE, BIOLOG, and BIODEG including over 25 different physical-chemical properties.	(Syracuse Research Corporation, 2004c)

Table 1 (continued). On-line sources of physical-chemical data.

[CASRN, Chemical Abstracts Registry Number; MW, molecular weight; BP, boiling point; MP, melting point; VP, vapor pressure; H, Henry's law constant; Koc, soil sorption coefficient; Kp, permeability constant; Kd, soil-water partition coefficient; Kow, octanol-water partition coefficient; pKa, dissociation constant; BCF, bioconcentration factor]

Title	Type of data provided	Reference
EXtension TOXicology NETwork (EXTOXNET) Pesticide Information Profiles	Appearance, MW, water solubility, solubility in other solvents, MP, VP, log Kow, adsorption coefficient, breakdown in soil and groundwater, breakdown in water, and breakdown in vegetation.	(University California-Davis and others, 2004)
Hazardous Substances Data Bank (HSDB)	Molecular formula, MW, color/form, odor, taste, BP, MP, critical temperature and pressure, density/specific gravity, dissociation constants, heat of combustion, heat of vaporization, log Kow, solubilities, surface tension, VP, viscosity, saturation concentration, specific heat of liquid, heat of fusion, and H.	(National Library of Medicine, 2004a)
Information System for Hazardous Organics in Water (ISHOW)	MP, BP, VP, water solubility, Kow, pKa.	(National Information Services Corporation, 1990b)
International Chemical Safety Cards	Physical state, appearance, BP, MP, relative density (water = 1), water solubility, VP, relative vapor density (air = 1), relative density of the vapor/air-mixture at 20°C, flashpoint, and auto-ignition temperature.	(National Institute for Occupational Safety and Health, 2004a)
International Uniform Chemical Information Database (IUCLID)	MP, BP, VP, density, various partition coefficients, solubility in different media, surface tension, flash point, flammability, oxidizing properties, pKa, viscosity.	(European Chemicals Bureau, 2001)
LogKow (KowWin)	Calculates log Kow and retrieves experimental log Kow data from an experimental database of 13,000 compounds.	(Syracuse Research Corporation, 2004d)
National Institute of Standards and Technology (NIST) Chemistry WebBook	H, enthalpy of formation, enthalpy of combustion, heat capacity, entropy, phase transition enthalpies and temperatures, VP, density, specific volume, viscosity, thermal conductivity, surface tension.	(National Institute of Standards and Technology, 2003)
Pesticide Reregistration Eligibility Decisions	MW, VP, degradation and mobility, field dissipation, bioaccumulation.	(U. S. Environmental Protection Agency, 2004f)
Office of Pollution Prevention & Toxics (OPPT) Chemical Fact Sheets	Physical state, MW, MP, BP, water solubility, density, vapor density, Koc, log Kow, VP, reactivity, flash point, H, BCF, odor threshold.	(U. S. Environmental Protection Agency, 2004e)
Oregon State University Extension Pesticide Properties Database	Pesticide movement rating, soil half-life, water solubility, soil Koc.	(Oregon State University Extension Service, 1994)
Organisation for Economic Co-operation and Development (OECD) Screening Information Data Set (SIDS) for High Production Volume Chemicals	MW, appearance, MP, BP, VP, log Kow, water solubility, H, pKa.	(United Nations Chemicals Programme, 2004)
PhysProp Database Demo	Molecular formula, MW, MP, BP, water solubility, log Kow, VP, pKa, H.	(Syracuse Research Corporation, 2004e)

Table 1 (continued). On-line sources of physical-chemical data.

[CASRN, Chemical Abstracts Registry Number; MW, molecular weight; BP, boiling point; MP, melting point; VP, vapor pressure; H, Henry's law constant; Koc, soil sorption coefficient; Kp, permeability constant; Kd, soil-water partition coefficient; Kow, octanol-water partition coefficient; pKa, dissociation constant; BCF, bioconcentration factor]

Title	Type of data provided	Reference
QSAR system	Computer system for estimation of physicochemical properties and ecotoxicological effects from chemical structures. The QSAR system has now been integrated into the ASTER program.	(U. S. Environmental Protection Agency, 1988)
Right to Know Hazardous Substance Fact Sheets	VP, flash point, water solubility.	(New Jersey Department of Health and Senior Services, 2004)
Risk Assessment Information System (RAIS) – Chemical-Specific Factors	Diffusivity in air (Di), diffusivity in water (Dw), Kp, Kd, H, MW, Koc, log Kow, water solubility, VP, MP, BP, radioactive half-life, fish bioaccumulation factor.	(U.S. Department of Energy, 2004)
SOLV-DB	MW, BP, freeze point, VP, specific gravity, surface tension, vapor density, flash point.	(National Center for Manufacturing Sciences, 1998)
Structure and Nomenclature Search System (SANSS)	Molecular formula, MW, chemical structure diagram, synonyms and trade names.	(National Information Services Corporation, 1999)
Toxic Substances Control Act Test Submissions (TSCATS)	Part of the Chemical Information System. TSCATS enables users to identify and obtain copies of unpublished health and safety studies submitted to the EPA. Physical-chemical data include pKa, H, Kow, VP, water solubility, and photolysis.	(National Information Services Corporation, 2004)

Table 2. Selected literature sources of physical-chemical data.

[MP, melting point; BP, boiling point; pKa, dissociation constant; H, Henry's law constant; BCF, bioconcentration factor; Koc, soil sorption coefficient; Kow, octanol-water partition coefficient; VP, vapor pressure; MW, molecular weight]

Title	Type of data provided	Reference
Agrochemicals desk reference environmental data	Environmental and physical/chemical data on more than 200 compounds, including pesticides, herbicides, and fungicides.	(Montgomery, 1993)
CRC Handbook of chemistry and physics	Water solubility, molecular formula, MP, BP, density, physical state.	(Lide, 2003)
Ground water desk reference	Diffusivity in water, pKa, H, BCF, log Koc, log Kow, solubility in water and organics, environmental fate, and some toxicity data.	(Montgomery, 2000)
Handbook of property estimation methods for chemicals, environmental and health sciences	Water solubility, VP, H, log Kow, log Koc, BCF and biomagnification factor in aquatic environments, reactivity or persistence information such as hydrolysis, biodegradation, and photoreactions.	(Boethling and Mackay, 2000)
Handbook of environmental data on organic chemicals	VP, water solubility, log Kow, H, biodegradation, oxidation.	(Verschueren, 1996)
Illustrated handbook of physical-chemical properties and environmental fate for organic chemicals, vol. I-III	Log Koc, log Kow, water solubility, VP, H, BCF, pKa, half life.	(Mackay and others, 1991-1993)
Measurement of Henry's Law constant as function of temperature and salinity for the low temperature range	H	(Dewulf and others, 1995)
Merck Index: An Encyclopedia of chemicals, drugs, & biologicals	BP, density, MW, physical state, chemical structure, some toxicity data.	(O'Neil and others, 2001)
Pesticides in the atmosphere-distribution, trends, and governing factors	water solubility, VP, H.	(Majewski and Capel, 1995)
Transport, behavior, and fate of volatile organic compounds in streams	H, log Koc, hydrolysis half-life.	(Rathbun, 1998)
Using the static headspace method to determine Henry's Law constants	H	(Robbins and others, 1993)

Table 3. Sources of human toxicity data.

[MCL, Maximum Contaminant Level; HA, Health Advisory, DWEL, Drinking Water Equivalent Level; LOEL, Lowest Observable Effect Level; NOAEL, No Observable Adverse Effect Level; RfD, reference dose; PEL, Permissible Exposure Limit; TLV, Threshold Limit Value; RfC, reference concentration; NOEL, No Observable Effect Level; MRL, Minimal Risk Level; LC50, Lethal Concentration 50%; REL, Recommended Exposure Limits]

Title	Type of data provided	Reference
Agency for Toxic Substances and Disease Registry (ATSDR) Toxicological Profiles	Toxicology data for hazardous substances found at National Priorities List sites. Profiles contain information on (a) health effects data including genotoxicity, toxicokinetics, and mechanisms of action, (b) physical-chemical properties, (c) production and use information, and (c) potential for human exposure.	(Agency for Toxic Substances and Disease Registry, 2004a)
Chemical Carcinogenesis Research Information System (CCRIS)	A summary of carcinogenicity, mutagenicity, tumor promotion, and tumor inhibition test results from the literature.	(National Cancer Institute, 2004)
Chemical Information System	Human toxicity data available from CCRIS, IRIS, MEDLINE, NIOSHTIC, RISKLINE, RTECS, and TSCATS (see these listings for more details). Subscription necessary (free 30 day trial).	(U. S. Environmental Protection Agency, 2004a)
Drinking Water Regulations and Health Advisories	MCL, Maximum Contaminant Level Goal (MCLG), HA, DWEL, cancer risk, cancer classification. Supporting technical documentation for the health advisories is available and can be ordered for a fee at http://www.epa.gov/OST/orderpubs.html	(U. S. Environmental Protection Agency, 2004a)
EXtension TOXicology NETwork (EXTOXNET) Pesticide Information Profiles	Summaries of acute, chronic, reproductive, teratogenic, mutagenic, carcinogenic, and organ toxicity studies from the literature for pesticides. Citations are listed. Also HA, DWEL, LOEL, NOAEL, RfD, PEL, TLV, and MCL values with citations. Does not provide supporting information.	(University California-Davis and others, 2004)
Forest Service Pesticide Fact Sheets	Acute oral, dermal, and inhalation toxicity in terrestrial animals; primary irritation score; primary eye irritation; chronic toxicity including carcinogenicity, developmental toxicity, reproductive toxicity, and mutagenicity; human health effects including acute toxicity/poisoning and chronic toxicity.	(U.S. Department of Agriculture, 2004)
Hazard Assessment of the Organophosphates	Descriptive neurological, developmental, and reproductive toxicology data, and NOEL and LOEL values for organophosphate pesticides.	(U. S. Environmental Protection Agency, 1998)
Hazardous Substances Data Bank (HSDB)	Contains summaries of human and other animal toxicity studies found in the literature with citations. Describes acute toxicity, chronic toxicity, carcinogenicity, mutagenicity, teratogenicity, occupational exposure effects.	(National Library of Medicine, 2004a)
HazDat	Provides access to information on the release of hazardous substances from Superfund sites or from emergency events and on the effects of hazardous substances on the health of human populations.	(Agency for Toxic Substances and Disease Registry, 2002)

Table 3 (continued). Sources of human toxicity data.

[MCL, Maximum Contaminant Level; HA, Health Advisory, DWEL, Drinking Water Equivalent Level; LOEL, Lowest Observable Effect Level; NOAEL, No Observable Adverse Effect Level; RfD, reference dose; PEL, Permissible Exposure Limit; TLV, Threshold Limit Value; RfC, reference concentration; NOEL, No Observable Effect Level; MRL, Minimal Risk Level; LC50, Lethal Concentration 50%; REL, Recommended Exposure Limits]

Title	Type of data provided	Reference
Health Effects Assessment Summary Tables (HEAST)	Lists RfD, and RfC, slope factor, unit risk values, and cancer classification, but does not provide supporting information.	(U. S. Environmental Protection Agency, 1997b)
Integrated Risk Information System (IRIS)	RfD, RfC, slope factor, cancer classification. Substantial supporting information and documentation also provided.	(U. S. Environmental Protection Agency, 2003b)
International Agency for Research on Cancer (IARC) Evaluations of Carcinogenicity to Humans	Contains summaries of human and other animal carcinogenicity studies from the literature and assigns a cancer class.	(International Agency for Research on Cancer, 2004)
International Chemical Safety Cards	Acute hazards and symptoms from inhalation, dermal, ocular, and oral exposure, and occupational exposure limits including TLV, PEL, REL, and Immediately Dangerous to Life and Health (IDLH). Some values have citations, but not all.	(National Institute for Occupational Safety and Health, 2004a)
International Toxicity Estimates for Risk (ITER) database	A compendium of EPA RfD, RfC, and oral and inhalation cancer risk values, ATSDR MRLs, Health Canada values, and values from other sources (e.g., industry, academia) with citations.	(TERA (Toxicology Excellence for Risk Assessment) and Concurrent Technologies Corporation, 2004)
International Uniform Chemical Information Database (IUCLID)	Acute oral toxicity, acute inhalation toxicity, acute dermal toxicity, acute toxicity other routes, skin irritation, eye irritation, sensitization, repeated dose toxicity, genetic toxicity <i>in vitro</i> and <i>in vivo</i> , carcinogenicity, reproductive toxicity, developmental toxicity/teratogenicity.	(European Chemicals Bureau, 2001)
MEDLINE/PubMed	Part of the Chemical Information System. PubMed includes over 14 million citations for biomedical articles back to the 1950's. These citations are from MEDLINE and additional life science journals.	(National Library of Medicine, 2004b)
MRL values	MRL values and toxic endpoints/effects. Substantial supporting information and documentation also provided.	(Agency for Toxic Substances and Disease Registry, 2004b)
National Toxicology Program (NTP) Report on Carcinogens	NTP human cancer classification and a summary of carcinogenicity studies from the literature with citations.	(National Toxicology Program, 2002)
NIOSH Pocket Guide	REL and PEL values and symptoms of exposure. Does not provide supporting information.	(National Institute for Occupational Safety and Health, 2003)
NIOSH TIC	Part of the Chemical Information System. NIOSHTIC-2 is a bibliographic database of occupational safety and health publications, documents, grant reports, and other communication products.	(National Institute for Occupational Safety and Health, 2004b)

Table 3 (continued). Sources of human toxicity data.

[MCL, Maximum Contaminant Level; HA, Health Advisory, DWEL, Drinking Water Equivalent Level; LOEL, Lowest Observable Effect Level; NOAEL, No Observable Adverse Effect Level; RfD, reference dose; PEL, Permissible Exposure Limit; TLV, Threshold Limit Value; RfC, reference concentration; NOEL, No Observable Effect Level; MRL, Minimal Risk Level; LC50, Lethal Concentration 50%; REL, Recommended Exposure Limits]

Title	Type of data provided	Reference
Office of Pollution Prevention & Toxics (OPPT) Chemical Fact Sheets	Summaries of animal and human studies from the literature of acute toxicity, subchronic and chronic toxicity, carcinogenicity, genotoxicity, developmental and reproductive toxicity, and neurotoxicity with citations.	(U. S. Environmental Protection Agency, 2004e)
Organisation for Economic Co-operation and Development (OECD) Screening Information Data Set (SIDS) for High Production Volume Chemicals	Summaries from the literature of acute oral, inhalation, and dermal toxicity; dermal, ocular, and respiratory irritation; sensitization; chronic toxicity; genetic toxicity <i>in vivo</i> and <i>in vitro</i> ; carcinogenicity; reproductive and developmental toxicity; teratogenicity; experience with human exposure, all with citations. Also, occupational exposure limits from a number of countries.	(United Nations Chemicals Programme, 2004)
Pesticide Reregistration Eligibility Decisions	Summaries of studies of acute toxicity, subchronic toxicity, chronic toxicity and carcinogenicity, developmental and reproductive toxicity, mutagenicity, and metabolism, with citations. Dose-response assessment including RfD values, q1* (slope factors), dermal absorption, and cancer classification. Also dietary, drinking water, and occupational risk characterization.	(U. S. Environmental Protection Agency, 2004f)
Reference Dose Tracking Report	Pesticide RfD, NOEL, LEL, carcinogenicity, and laboratory animal effects. Does not provide supporting information.	(U. S. Environmental Protection Agency, 1997c)
Registry of Toxic Effects of Chemical Substances (RTECS)	RTECS is a compendium of data extracted from the open scientific literature. Six types of toxicity data are included: (1) primary irritation; (2) mutagenic effects; (3) reproductive effects; (4) tumorigenic effects; (5) acute toxicity; and (6) other multiple-dose toxicity. Specific numeric toxicity values such as LD50, LC50, and toxic doses and concentrations are noted as well as species studied and route of administration used. For each citation, the bibliographic source is listed.	(MDL Information Systems Inc., 2004)
Right to Know Hazardous Substance Fact Sheets	A short summary of acute and chronic health effects, cancer and reproductive hazards, and other long-term effects. Also occupational exposure limits from the Occupational Safety and Health Administration (OSHA), NIOSH, and American Conference of Industrial Hygienists (ACGIH). Citations and supporting information or documentation are not provided.	(New Jersey Department of Health and Senior Services, 2004)

Table 3 (continued). Sources of human toxicity data.

[MCL, Maximum Contaminant Level; HA, Health Advisory, DWEL, Drinking Water Equivalent Level; LOEL, Lowest Observable Effect Level; NOAEL, No Observable Adverse Effect Level; RfD, reference dose; PEL, Permissible Exposure Limit; TLV, Threshold Limit Value; RfC, reference concentration; NOEL, No Observable Effect Level; MRL, Minimal Risk Level; LC50, Lethal Concentration 50%; REL, Recommended Exposure Limits]

Title	Type of data provided	Reference
Risk Assessment Information System (RAIS) – toxicity values	A compendium of IRIS, HEAST, EPA Provisional Peer Reviewed Toxicity Values (PPRTVs), and other data when available. Citations and supporting information are provided. The toxicity values contained in this database were developed for use in risk evaluations and assessments utilizing methods presented in Risk Assessment Guidance for Superfund: Volume I - Human Health Evaluation Manual (RAGS).	(U.S. Department of Energy, 2004)
RISKLINE	Part of the Chemical Information System. RISKLINE includes bibliographic records and abstracts dealing with human and animal toxicology and carcinogenicity. The earliest records in the database date from 1970, the latest from 2001.	(National Information Services Corporation, 2001)
Scorecard	A list of human health effects, a summary of EPA's review of whether acute toxicity, chronic toxicity, neurotoxicity, developmental or reproductive toxicity, mutagenicity, carcinogenicity, ecotoxicity, and environmental fate data are available for high production volume chemicals. Also lists toxicity values including RfD, MCL, ingestion cancer risk value, National ambient air quality standard, RfC, and inhalation cancer risk value, and links to other sources of information.	(Environmental Defense, 2003)
SIRI Material Safety Data Sheets (MSDS)	Brief descriptions of acute and chronic human health effects.	(University of Vermont, 2004)
Substance Registry System	Regulatory information and hyperlinks to other sources of data (including toxicity data from sources such as IARC, ATSDR, IRIS, NIOSH, NTP, EPA Office of Water Drinking Water Regulations and Health Advisories, TERA/ITER and TSCATS). "The SRS serves as the nucleus for linking information about substances regulated by the EPA". Incorporates the Chemical Registry System, which is no longer in use.	(U. S. Environmental Protection Agency, 2004g)
Toxic Substances Control Act Test Submissions (TSCATS)	Part of the Chemical Information System. TSCATS enables users to identify and obtain copies of unpublished health and safety studies submitted to the EPA. Toxicity data include information on acute toxicity; biochemical interactions/mechanism of action; chronic toxicity; carcinogenicity; chronic toxicity - combined chronic toxicity/carcinogenicity; chronic toxicity - cell transformation, dermal irritation; dermal sensitization; eye irritation; epidemiology study; genotoxicity; industrial hygiene; neurotoxicity; reproduction/fertility effects; teratogenicity; subchronic toxicity; and tissue concentration determination.	(National Information Services Corporation, 2004)

Table 4. Sources of aquatic toxicity data.

[LC50, Lethal Concentration 50%; EC50, Effective Concentration 50%; LOAEL; Lowest Observable Adverse Effect Level; NOAEL, No Observable Adverse Effect Level; BCF, bioconcentration factor]

Title	Type of data provided	Reference
Aquatic Toxicity Information Retrieval (AQUIRE)	In 1995, the AQUIRE database became a component of the ECOTOX database (see ECOTOX listing).	(U. S. Environmental Protection Agency, 2004d)
AQUATOX	AQUATOX is a simulation model for aquatic systems that predicts the fate of various pollutants, such as nutrients and organic chemicals, and their effects on the ecosystem, including acute and chronic toxicity toward fish, invertebrates, and aquatic plants.	(U. S. Environmental Protection Agency, 2004b)
ASsessment Tools for the Evaluation of Risk (ASTER)	ASTER is an integration of the AQUIRE toxic effects database and the QSAR system (see table 1 for QSAR system listing). When empirical data are not available mechanistically-based predictive models are used to estimate ecotoxicology endpoints, chemical properties, biodegradation, and environmental partitioning. Note: Due to security restrictions, ASTER is currently not publicly available. Technical support staff will conduct an ASTER search for persons affiliated with governmental offices.	(U. S. Environmental Protection Agency, 2004c)
Building, Assessing and Standardising Information on the Atlantic Coasts (BASIC) toxicity database	Contains information on the aquatic toxicity of a number of hazardous substances. When available, UK, US, Canadian, EU, and other guidelines are given.	(United Kingdom Department for Environment, 2001)
California Wildlife Exposure Factor and Toxicity Database (CAL/ECOTOX)	Toxicity data (sublethal behavioral effects, sublethal organ/system effects, LD50, LC50, LOAEL, NOAEL, mortality in the field, biomarkers such as changes in brain cholinesterase, reproductive toxicity, developmental effects, BCF, cellular/biochemical effects) for some California mammals, birds, amphibians, and reptiles.	(California Environmental Protection Agency, 1999)
Canadian environmental quality guidelines: Summary of existing Canadian environmental quality guidelines	Canadian water quality guidelines for freshwater and marine aquatic life. Supporting information and documentation also provided.	(Canadian Council of Ministers of the Environment, 2002)
Chemical Information System	Subscription necessary (free 30 day trial). Aquatic toxicity data available from AQUIRE, Registry of Toxic Effects of Chemical Substances (RTECS) (table 3), and Toxic Substances Control Act Test Submissions (TSCATS) (table 3).	(National Information Services Corporation, 2003)
Columbia Environmental Research Center (CERC) Acute Toxicity Database	Summarizes the results from aquatic acute toxicity tests conducted by the Columbia Environmental Research Center.	(U. S. Geological Survey, 1986)
Ecological Structure Activity Relationships (ECOSAR)	Software that predicts the toxicity of industrial chemicals to aquatic organisms such as fish, invertebrates, and algae by using Structure Activity Relationships.	(U. S. Environmental Protection Agency, 2000)

Table 4 (continued). Sources of aquatic toxicity data.

[LC50, Lethal Concentration 50%; EC50, Effective Concentration 50%; LOAEL; Lowest Observable Adverse Effect Level; NOAEL, No Observable Adverse Effect Level; BCF, bioconcentration factor]

Title	Type of data provided	Reference
ECOTOXicology (ECOTOX)	Chemical toxicity information for aquatic and terrestrial plants and animals. Single chemical toxicity data from three U.S. Environmental Protection Agency (USEPA) ecological effects databases; AQUIRE, Terrestrial Toxicity Information (TERRETOX), and PHYTO TOXicity (PHYTOTOX).	(U. S. Environmental Protection Agency, 2004d)
EValuation and Interpretation of Some Test Results in AQUIRE (EVISTRA)	The EVISTRA database is not yet available, but will present results that (a) were obtained from aquatic toxicity tests on selected pollutants and (b) were evaluated for eligibility and uncertainty (and interpreted when necessary).	(U. S. Environmental Protection Agency, 2003a)
Fathead minnow database	Results of 617 acute LC50 values and 225 associated behavioral assessments, 72 joint toxic action experiments with the fathead minnow, and physiological response of rainbow trout (also called Fish Acute Toxicity Studies (FATS)) for 17 compounds.	(U. S. Environmental Protection Agency, 1997a)
Handbook of acute toxicity of chemicals to fish and aquatic invertebrates	Summaries of toxicity tests conducted at Columbia National Fisheries Research Laboratory 1965-1978, including 1,578 acute toxicity tests on 271 chemicals against 28 species of fish and 30 species of invertebrates.	(Johnson and Finley, 1980)
Hazardous Substances Data Bank (HSDB)	Summaries of aquatic toxicity tests (LC50 values) from the literature and citations.	(National Library of Medicine, 2004a)
International Uniform Chemical Information Database (IUCLID)	Toxicity to fish, aquatic invertebrates, aquatic plants, and microorganisms.	(European Chemicals Bureau, 2001)
LC50 Software Model	LC50 is a program that estimates LC50 values using the Trimmed Spearman-Kärber Method.	(U. S. Environmental Protection Agency, 1999)
National Recommended Water Quality Criteria	Freshwater and saltwater Criteria Maximum Concentration (CMC) and Criterion Continuous Concentration (CCC) values. Supporting information and documentation also provided.	(U. S. Environmental Protection Agency, 2002a)
Office of Pollution Prevention & Toxics (OPPT) Chemical Fact Sheets	LC50 values from the literature. Limited supporting information.	(U. S. Environmental Protection Agency, 2004e)
Organisation for Economic Co-operation and Development (OECD) Screening Information Data Set (SIDS) for High Production Volume Chemicals	Acute and chronic toxicity to fish and aquatic invertebrates. Includes supporting information and documentation.	(United Nations Chemicals Programme, 2004)
PAN Pesticides Database	Includes 223,853 aquatic toxicity results from USEPA's AQUIRE database. These data can be searched by species, chemical or effect.	(Orme and Kegley, 2004)

Table 4 (continued). Sources of aquatic toxicity data.

[LC50, Lethal Concentration 50%; EC50, Effective Concentration 50%; LOAEL; Lowest Observable Adverse Effect Level; NOAEL, No Observable Adverse Effect Level; BCF, bioconcentration factor]

Title	Type of data provided	Reference
Pesticide ecotoxicity database	Environmental endpoints for over 15,000 toxicity studies that measure the impact of pesticides on fish, birds, insects, amphibians, wild mammals, plants, and invertebrates for over 630 pesticide active ingredients.	(U. S. Environmental Protection Agency, 2002b)
Pesticide toxicity index for freshwater aquatic organisms	Aquatic organism EC50 and LC50 values for National Water-Quality Assessment Program (NAWQA) pesticides.	(Munn and Gilliom, 2001)
Summary of published aquatic toxicity information and water-quality criteria for selected volatile organic compounds	USEPA freshwater acute criteria/guidelines, USEPA freshwater chronic criteria/guidelines, Canadian water-quality guidelines, LC50, EC50, Lowest Observable Effect Concentration (LOEC), Maximum Acceptable Threshold Concentration (MATC), No Observable Effect Concentration (NOEC), and endpoint effects for NAWQA VOCs, all with citations.	(Rowe and others, 1997)
Toxicity/Residue database	More than 3,000 effect and no-effect endpoints for survival, growth and reproductive parameters for invertebrates, fish and aquatic life-stage of amphibians. Data were abstracted from approximately 500 literature references on approximately 200 chemicals and 190 freshwater and marine test species.	(U. S. Environmental Protection Agency, 2003c)
Toxicological benchmarks for screening potential contaminants of concern for effects on aquatic biota	Acute and chronic National Ambient Water Quality Criteria (NAWQC), Final Acute Values (FAV), Secondary Acute Values (SAV), Chronic Values (CV), Secondary Chronic Values (SCV), and Effective Concentration 20% (EC ₂₀) values. Includes supporting information and documentation.	(Suter and Tsao, 1996)

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