

US EPA and Other Organization Tools for Chemicals Assessment and Design

The US Environmental Protection Agency and other organizations have developed an extensive array of tools to assist in chemicals prioritization and assessment. Some of these tools, along with website links are listed below.

Many of the EPA tools and information about EPA's pollution prevention, chemical assessment, green chemistry and Design for Environment programs are available on the following EPA websites: <http://www.epa.gov/oppt/tools/dsalpha.htm> and <http://www.epa.gov/epahome/Data.html>

Chemical Toxicity Data

<http://www.epa.gov/iris/>

IRIS Database. IRIS is a database of human health effects that may result from exposure to various substances found in the environment. IRIS was initially developed for EPA staff in response to a growing demand for consistent information on chemical substances for use in risk assessments, decision-making and regulatory activities.

<http://toxnet.nlm.nih.gov/>

Toxnet. Toxnet is a series of databases on chemical toxicity hosted by the National Institutes of Medicine which allows multiple searching options.

http://www.epa.gov/8e_triag/

EPA Triage Database. Triage is a searchable database of scientific studies on the health and environmental effects of toxic chemicals related to Section 8(e) of TSCA.

<http://www.epa.gov/tri/index.htm>

http://www.epa.gov/enviro/html/tris/tris_query.html

Toxics Release Inventory Resources. The Toxics Release Inventory (TRI) is a publicly available EPA database that contains information on toxic chemical releases and other waste management activities reported annually by certain covered industry groups as well as federal facilities.

<http://www.rtknet.org/tsc/>

TSCATS. TSCATS (Toxic Substances Control Act Test Submissions) is an online index to unpublished, non-confidential studies covering chemical testing results and adverse effects of chemicals on health and ecological systems. The studies are submitted by U.S. industry to EPA under several sections of the Toxic Substance Control Act (TSCA). There are four types of documents in the database: Section 4 chemical testing results, Section 8(d) health and safety studies, Section 8(e) substantial risk of injury to health or the environment notices, and voluntary documents submitted to EPA known as a For Your Information (FYI) notice.

<http://www.scorecard.org>

The Scorecard Database provides information on chemical releases, risk prioritization of substances and other relevant information for chemicals and facilities.

<http://ecb.jrc.it/>

European Chemicals Bureau databases. The European Chemicals Bureau is the European Commission focal point for data and the assessment procedure on dangerous chemicals. Once REACH comes into force, many of these capacities will be transferred to a new Chemicals Agency in Helsinki.

Exposure Assessment Tools

The EPA Office of Pollution Prevention and Toxics (OPPT) has developed several exposure assessment methods, databases, and predictive models to help in evaluating:

- what happens to chemicals when they are used and released to the environment; and
- how workers, the general public, consumers and the aquatic ecosystems may be exposed to chemicals.

See: <http://www.epa.gov/oppt/exposure/> for the list of tools and descriptions of them.

These tools may be helpful when appropriate monitoring data are not available or need to be supplemented, and in considering potential exposure when designing and selecting products and processes; and evaluating pollution prevention opportunities.

The results of an exposure assessment are generally combined with a hazard assessment (potential for a chemical to cause adverse health or environmental effects).

http://www.hc-sc.gc.ca/ewh-semt/alt_formats/hecs-sesc/pdf/contaminants/existsub/greatest_potential_human_exposure.pdf

Health Canada Proposal for Priority Setting for Existing Substances on the Domestic Substances List under the Canadian Environmental Protection Act, 1999: Greatest Potential for Human Exposure. This report describes a proposed priority setting process of existing substances in Canada. A stakeholder meeting was convened to discuss the Complex Exposure Model (comET). For more on the Canadian chemical substances review process see <http://www.chemicalsubstanceschimiques.gc.ca/>

Hazard and Risk Assessment Tools

<http://www.epa.gov/hpvis/index.html>

The High Production Volume Information System (HPVIS) provides complete and easy access to technical health and environmental effect information on chemicals that are manufactured in exceptionally large amounts. Information in this database is submitted through EPA's High Production Volume (HPV) Challenge Program. HPVIS allows users to search for summary information, test plans, and new data on high production volume chemicals as they are developed.

PBT Profiler

<http://www.pbtprofiler.net/>

EPA has developed an evaluation tool, the PBT Profiler, which predicts PBT potential of chemicals. The PBT Profiler estimates environmental persistence (P), bioconcentration potential (B), and aquatic toxicity (T) of discrete chemicals based on their molecular structure. It is Internet-based and there is no cost for use. The user enters a chemical using the [Chemical Abstract Service Registry Number \(CASRN\)](#). If the chemical is in the accompanying database of more than 100,000 chemicals, the structure is retrieved and entered into the model. A drawing program is also available so that the user can draw and enter the structure or the structure can be entered as a line notation using the Simplified Molecular Input Line Entry System (SMILES). The PBT Profiler is a web-based evaluation tool that may be valuable for those developing new chemicals or considering the use of new chemicals.

<http://www.epa.gov/oppt/newchems/tools/21ecosar.htm>

ECOSAR (Ecological Structure Activity Relationships) is a personal computer software program that is used to estimate the toxicity of chemicals used in industry and discharged into water. The program predicts the toxicity of industrial chemicals to aquatic organisms such as fish, invertebrates, and algae by using Structure Activity Relationships (SARs). The program estimates a chemical's acute (short-term) toxicity and, when available, chronic (long-term or delayed) toxicity.

<http://www.epa.gov/oppt/newchems/tools/oncologic.htm>

OncoLogic is a desktop computer program that evaluates the likelihood that a chemical may cause cancer.

<http://international.vrom.nl/pagina.html?id=7386>

Netherlands Ministry of Housing, Spatial Planning and Environment Quick Scan Process. The Quick Scan Process is a rapid qualitative risk assessment and prioritization process for chemicals in commerce. It provides a simple way to categorize and prioritize chemicals based on a minimal data set.

<http://glwww.mst.dk/chemi/01050000.htm>

The Danish EPA has developed an advisory list for self-classification of dangerous substances including 20,624 substances. The substances have been identified by means of computer models, so-called QSAR models (Quantitative Structure-Activity Relationship)

<http://www.coshh-essentials.org.uk/>

Developed by the UK Health and Safety Executive, COSHH Essentials provides advice on controlling the use of chemicals for a range of common tasks, eg mixing, or drying.

Safer Chemistry Design Tools

<http://www.epa.gov/oppt/newchems/pubs/sustainablefutures.htm>

Many of the EPA initiatives on sustainable chemistry fall under the Sustainable Futures (SF) program - an approach that encourages pollution prevention in new chemical development through the transfer of OPPT's chemical risk screening methodologies. The

[Federal Register Notice \[PDF\]](#) announcing SF has detailed information on what is required of participants and the mechanism for expedited review available; and discusses factors EPA will consider when determining eligibility of participants for the expedited review.

<http://www.cleangredients.org/>

Green Blue Institute Clean Gradients Database. CleanGradients™ is being developed as an online database of institutional and industrial (I&I) cleaning ingredients — a one-stop-shop for green formulation. The database aligns broad environmental and human health goals with the cleaning product industry's business objectives and will support formulators in formulating products with human and environmental health benefits, whether to meet corporate internal objectives, more stringent regulations, voluntary product recognition programs or national and international eco-label.

<http://www.epa.gov/greenchemistry/pubs/tools.html>

The Green Chemistry Expert System (GCES) allows users to build a green chemical process, design a green chemical, or survey the field of green chemistry. The system is equally useful for new and existing chemicals and their synthetic processes. It includes extensive documentation.

The GCES features are contained in five modules:

- The Synthetic Methodology Assessment for Reduction Techniques (SMART) <http://www.epa.gov/greenchemistry/pubs/smart.html> module quantifies and categorizes the hazardous substances used in or generated by a chemical reaction, based on information entered by the user. Reactions can be modified in the SMART module and re-evaluated to optimize their green nature.
- The Green Synthetic Reactions module provides technical information on green synthetic methods.
- The Designing Safer Chemicals module includes guidance on how chemical substances can be modified to make them safer; it is organized by chemical class, properties, and use.
- The Green Solvents/Reaction Conditions module contains technical information on green alternatives to traditional solvent systems. This module also allows users to search for green substitute solvents based on physicochemical properties.
- The Green Chemistry References module allows the user to obtain additional information using a number of search strategies.

<http://fusion.stolaf.edu/gca/>

The Green Chemistry Assistant, a web application currently under development at St. Olaf college, is based on the SMART module of the Green Chemistry Expert System <http://www.epa.gov/gcc/pubs/tools.html#expert> . It allows improved input of reaction data and a more thorough analysis of overall process mass inputs and outputs. The GCA does not yet incorporate the hazard tiers from the GCES SMART module.

Alternatives Assessment Methodologies

http://www.turi.org/library/turi_publications/five_chemicals_study

The Massachusetts Toxics Use Reduction Institute has developed an Alternatives Assessment Process Guidance for its analysis of substitutes to five chemicals in Massachusetts.

EPA has partnered with industry for several projects aimed at assessing alternative chemicals particular to specific industrial sectors. Included in these are the Formulator Program <http://www.epa.gov/dfepubs/projects/formulat/index.htm>, the Furniture and Flame Retardancy Partnership <http://www.epa.gov/dfepubs/projects/flameret/index.htm>, and the Flame Retardants in Printed Circuit Boards Partnership <http://www.epa.gov/dfepubs/projects/pcb/index.htm>.

<http://www.greenchemex.org/>

Green Chemistry Exchange is a web-based database of green chemistry resources.

http://www.kemi.se/templates/PRIOEngframes_4144.aspx

Swedish Chemicals Inspectorate PRIO Program. PRIO is a web-based tool intended to be used to preventively reduce risks to human health and the environment from chemicals. PRIO replaces the Swedish Chemicals Inspectorate's Observation (OBS) list. The aim of PRIO is to facilitate in the assessment of health and environmental risks of chemicals so that people who work as environmental managers, purchasers and product developers can identify the need for risk reduction. To achieve this PRIO provides a guide for decision-making that can be used in setting risk reduction priorities.

<http://glwww.mst.dk/chemi/01040000.htm>

The Danish List of Undesirable Substances is a list of chemicals of concern that the government believes should be avoided to the extent feasible in commerce. EPA's Design for Environment Initiative has developed numerous partnerships to examine alternatives to various chemicals and uses of chemicals in a variety of product types. For general information see www.epa.gov/dfepubs