

## **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: [www.epa.gov/oppt](http://www.epa.gov/oppt) 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/](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](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 TSCATS (Toxic Substances Control Act Test Submissions) is an online index to unpublished, nonconfidential studies covering chemical testing results and adverse effects of chemicals on health and ecological systems.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://www.cleangredients.org/>

Green Blue Institute Clean Gradients Database. CleanGredients™ 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://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.

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).

OPPT uses these tools in a [tiered approach to exposure assessment](#). The exposure assessment tools have been grouped by Specialized Priority Setting Tools, Screening Level Tools, and Higher Tier Tools. The three categories of tools can be used together in a tiered approach to efficiently assess potential exposures to chemicals.

[Specialized Priority Setting Tools](#) use standardized criteria and exposure models, and hazard information. These Tools are designed to:

- rapidly compare large numbers of chemicals by ranking them on the basis of relative risk and/or exposure using standardized criteria; and
- rank concerns broadly, and thus are not intended to provide detailed and accurate exposure assessments.

These are useful for evaluating a large number (hundreds, thousands) of chemicals for potential exposures, these tools can help in identifying chemicals and issues for further review. Specialized Priority Setting Tools include:

#### [Source Ranking Database](#)

- performs a systematic screening-level review of over 12,000 potential indoor pollution sources to identify high-priority product and material categories for further evaluation
- can also identify the products that have contained a specific chemical.

#### [Use Cluster Scoring System](#)

- identifies and screens clusters of chemicals ("use clusters") that are used to perform a particular task. A use cluster is a set of chemicals that may be substituted for one another in performing a given task
- identifies clusters of potential concern and provides an initial ranking of chemicals using human and environmental hazard and exposure data from a number of sources.

[Screening Level Tools](#) use readily available data and simple models, and are designed to:

- require minimal data entry;
- quickly screen release and exposure potential and "bin" chemicals by priority for future work; and
- estimate conservative (i.e., high or perhaps higher than actual) values of release and exposure.

Screening Level Tools include:

### [Chemical Screening Tool For Exposures And Environmental Releases](#)

- estimates occupational inhalation and dermal exposure to a chemical during industrial and commercial manufacturing, processing, and use operations involving the chemical.
- estimates releases of a chemical to air, water, and land that are associated with industrial and commercial manufacturing, processing, and use of the chemical.

### [Exposure, Fate Assessment Screening Tool \(EFAST\)](#)

- provides screening-level estimates of the concentrations of chemicals released to air, surface water, landfills, and from consumer products.
- estimates provided are potential inhalation, dermal and ingestion dose rates resulting from these releases.
- modeled estimates of concentrations and doses are designed to reasonably overestimate exposures, for use in screening level assessment.

### [Estimation Program Interface \(EPI\) Suite](#)

- estimates physical/chemical properties, environmental fate and transport, and includes estimation programs for LogKOW, KOC, Atmospheric Oxidation Potential, Henry's Law Constant, Water Solubility, Melting Point, Boiling Point, Vapor Pressure, Biodegradation, Bioconcentration Factor, Hydrolysis, Sewage Treatment Plant Removal, Fugacity Modeling, and Multimedia Modeling.

### [ReachScan](#)

- estimates surface water chemical concentrations at drinking water utilities downstream from industrial facilities.

**[Higher Tier Tools](#)** use detailed data and more sophisticated models and are designed to:

- be closely tailored to (i.e., simulate) the exposure scenario of concern; and
- produce results with a higher level of accuracy.

These tools are complex and often require substantial, detailed data as input to the model. Where possible, data sets and default values are included with the model. These tools are much more complex and require advanced skills. They include:

### [Internet Geographical Exposure Modeling System \(IGEMS\)](#)

- brings together in one system several EPA environmental fate and transport models and some of the environmental data needed to run them.
- includes models and data for ambient air, surface water, soil, and ground water, and makes the models much easier to use than their stand-alone counterparts.

- will have graphics and Geographical Information System (GIS) capabilities for displaying environmental modeling results.

### [Multi-Chamber Concentration And Exposure Model \(MCCEM\)](#)

- estimates average and peak indoor air concentrations of chemicals released from products or materials in houses, apartments, townhouses, or other residences. The data libraries contained in MCCEM are limited to residential settings. However, the model can be used to assess other indoor environments (e.g. schools, offices) if the user can supply the necessary inputs.
- estimates inhalation exposures to these chemicals, calculated as single day doses, chronic average daily doses, or lifetime average daily doses. (All dose estimates are potential doses; they do not account for actual absorption into the body.)

[http://www.hc-sc.gc.ca/ewh-semt/alt\\_formats/hecs-sesc/pdf/contaminants/existsub/greatest\\_potential\\_human\\_exposure.pdf](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).

### **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 are 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.turi.org/content/content/view/full/1125/>

Massachusetts Toxics Use Reduction Institute Pollution Prevention Options Analysis Tool (p2oasys). The Institute has developed P2OaSys to help companies determine whether the TUR options they are considering may have unforeseen negative environmental, worker or public health impacts. P2OASys allows companies to assess the potential environmental, worker, and public health impacts of alternative technologies aimed at reducing toxics use. The goal is more comprehensive and systematic thinking about the potential hazards posed by current and alternative processes identified during the TUR planning process.

<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://www.mst.dk/homepage/default.asp?Sub=http://www.mst.dk/udgiv/publications/2004/87-7614-477-1/html/default\\_eng.htm](http://www.mst.dk/homepage/default.asp?Sub=http://www.mst.dk/udgiv/publications/2004/87-7614-477-1/html/default_eng.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. Companies participating in SF receive the Pollution Prevention (P2) Framework (<http://www.epa.gov/oppt/p2framework/docs/p2model.htm>) risk screening methodologies, which OPPT developed and uses to evaluate new chemical notifications under TSCA.

<http://www.epa.gov/opptintr/greenchemistry/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 \(SMART\)](#) 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 [link to gces.html]. 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**

[www.turi.org](http://www.turi.org)

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

[http://www.kemi.se/templates/PRIOEngframes\\_\\_\\_4144.aspx](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://www.mst.dk/homepage/default.asp?Sub=http://www.mst.dk/udgiv/publications/2004/87-7614-477-1/html/default\\_eng.htm](http://www.mst.dk/homepage/default.asp?Sub=http://www.mst.dk/udgiv/publications/2004/87-7614-477-1/html/default_eng.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