

## **\*List of Resources for Hazard and Toxicological Screening and Research**

- A Resources to identify chemicals of concern**
- B Chemical toxicity**
- C Exposure assessment tools**
- D Hazard and risk assessment tools**
- E Safer chemistry design tools**

### **A. Resources to Identify Chemicals of Concern**

#### **CA Proposition 65**

[www.oehha.ca.gov/prop65.html](http://www.oehha.ca.gov/prop65.html)

'Prop 65' is a list of chemicals that have been confirmed by the state of California to be carcinogens and or reproductive toxins. Chemicals are listed by name and by CAS #

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#### **National Toxicology Program Report on Carcinogens**

[ntp.niehs.nih.gov/ntp/roc/toc11.html](http://ntp.niehs.nih.gov/ntp/roc/toc11.html)

NTP maintains a list of chemicals that are carcinogens, likely carcinogens or probable carcinogens.

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#### **Toxics Release Inventory Resources (TRI)**

[www.epa.gov/tri/index.htm](http://www.epa.gov/tri/index.htm)

TRI is a publicly available EPA database that contains information on toxic chemical release and other waste management activities reported annually by certain covered industry group as well as federal facilities.

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#### **Clean Air Act: Hazardous Air Pollutant List**

[www.epa.gov/ttn/atw/l88polls.html](http://www.epa.gov/ttn/atw/l88polls.html); [www.epa.gov/ttn/atw/pollutants/atwsmod.html](http://www.epa.gov/ttn/atw/pollutants/atwsmod.html)

US Congress amended the Federal Clean Air Act in 1990 to address a large number of air pollutants that are known to cause or may reasonably be anticipated to cause adverse effects to human health or adverse environmental effects. 188 specific pollutants and chemical groups were initially identified as hazardous air pollutants (HAPs), and the list has been modified over time.

### **SARA/EPCRA 3 7 3 List (TRI)**

[www.epa.gov/tri/chemical/index.htm](http://www.epa.gov/tri/chemical/index.htm)

Section 313 of the Emergency Planning and Community Right to Know Act (EPCRA) of 1986 was enacted to facilitate emergency planning, to minimize the effects of potential toxic chemical accidents, and to provide the public with information on releases of toxic chemicals in their communities. The current list contains 581 individually listed chemicals and 30 chemical categories.

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### **Clean Water Act Priority Pollutants List**

[oaspub.epa.gov/wqsdatabase/wqsi\\_epa\\_criteria.rep\\_parameter](http://oaspub.epa.gov/wqsdatabase/wqsi_epa_criteria.rep_parameter)

Section 307 of the CWA defines a list of 126 priority pollutants for which the US EPA must establish ambient water-quality criteria and effluent limitations.

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### **Comprehensive Environmental Response, Compensation, and Liability Act (CERCLA)**

[www.epa.gov/ceppo/pubs/title3.pdf](http://www.epa.gov/ceppo/pubs/title3.pdf)

List of over 800 chemicals from, Section 102 of CERCLA, Clean Water Act list of hazardous substances and priority pollutants. Any hazardous waste as defined under Section 3001 of Resource Conservation and Recovery Act; Clean Air Act list of hazardous air pollutants (HAPs) (Section 112); Toxic Substances Control Act list of imminent hazards (Section 7).

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### **Canadian Environmental Protection Act, 1999 (CEPA)**

[www.ec.gc.ca/CEPARRegistry/subs\\_list/Toxicupdate.cfm](http://www.ec.gc.ca/CEPARRegistry/subs_list/Toxicupdate.cfm)

Under CEPA substances that are determined to be 'toxic' are recommended for addition to the List of Toxic Substances (Schedule 1) of the Act.

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### **EU Risk Phrase**

[ec.europa.eu/environment/dansub/consolidated\\_en.htm](http://ec.europa.eu/environment/dansub/consolidated_en.htm)

Council Directive 67/548/EEC of 27 June 1967 on the approximation of laws, regulations and administrative provisions relating to the classification, packaging and labelling of dangerous substances. Annex I of the directive assigns Risk Phrases to chemical substances.

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### **European Commission's Community Strategy for Endocrine Disrupters**

[http://lec.europa.eu/environment/endocrine/strategy/substances\\_en.htm#priority\\_list](http://lec.europa.eu/environment/endocrine/strategy/substances_en.htm#priority_list)

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The European Commission (EC) has sponsored four reports that evaluate a set of 553 substances selected by experts and stakeholders for assessment for endocrine disruption. Each report addresses a subset of the total set based on priorities such as whether the chemicals are persistent, bioaccumulating or High Production Volume chemicals and/or whether or not there is already regulatory control of the chemical.

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### **WHO Water Quality Guidelines**

[www.who.int/water\\_sanitation\\_health/dwq/gdwq3/en/](http://www.who.int/water_sanitation_health/dwq/gdwq3/en/)

International standards for selected chemical, microbiology and other parameters.

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### **The Danish List of Undesirable Substances (LOUS)**

[glwww.mst.dk/homepage/default.asp?Sub=http://glwww.mst.dk/udgiv/publications/20087-7614-477-1/html/kolofon\\_eng.htm](http://glwww.mst.dk/homepage/default.asp?Sub=http://glwww.mst.dk/udgiv/publications/20087-7614-477-1/html/kolofon_eng.htm)

The Danish List of Undesirable Substances is a list of chemicals of concern that the government believes should be avoided feasible in commerce. Using a systematic analysis, substances are selected automatically if they meet some clear and defined criteria, for example, problematic classifications, because they are under suspicion for being PBT/vPvB (Persistent, Bioaccumulative, Toxic/very Persistent, very Bioaccumulative) or endocrine -disrupting.

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### **International Agency for Research on Cancer (IARC)**

[monographs.iarc.fr/index.php](http://monographs.iarc.fr/index.php)

IARC Monographs are the result of interdisciplinary working groups of expert scientists who review published studies and evaluate the weight of the evidence that an agent can increase the risk of cancer. Since 1971, more than 900 agents have been evaluated, of which approximately 400 have been identified as carcinogenic or potentially carcinogenic to humans.

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### **National Institute for Occupational Safety and Health (NIOSH) Carcinogen List**

[www.cdc.gov/niosh/npotocca.html](http://www.cdc.gov/niosh/npotocca.html)

NIOSH maintains a list of substances considered to be potential occupational carcinogens.

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### **Occupational Safety and Health Administration (OSHA)**

[www.osha.gov](http://www.osha.gov)

OSHA maintains a list of potential carcinogens. In addition, OSHA sets enforceable permissible

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exposure limits (PELS) to protect workers against the health effects of exposure to hazardous substances.

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### **EPA Water Disinfection By-Products with Carcinogenicity Estimates (DBPCAN)**

[www.epa.gov/ncct/dsstox/sdf\\_dbpcan.html](http://www.epa.gov/ncct/dsstox/sdf_dbpcan.html)

The DBPCAN database contains predicted estimates of carcinogenic potential for 209 chemicals detected in finished drinking water samples having undergone water disinfection treatment.

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### **PBT Profiler**

[www.pbtprofiler.net/](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.

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### **Health & Safety Executive (HSE) Direct**

[www.hse.gov.uk/legislation/services.11tm](http://www.hse.gov.uk/legislation/services.11tm)

The Health and Safety Commission is responsible for health and safety regulation in Great Britain. HSE Direct is a subscription service providing full-text access to the full range of HSE guidance publications as well as the consolidated and annotated text of health and safety legislation and recent legislative changes. It includes a 'Stop- Press' feature which informs the user of very recent legislative changes. HSE direct provides full-text versions of HSE Legal Services material (Approved Codes of Practice, 'L' series, Codes of Practice and HSR series); HSE forms; European Directives; Safety, Health and Environment cases; and summaries of British Standards. Users can choose from either 'day ticket' access or regular subscription options.

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### **CA Toxic Air Contaminants List**

[www.arb.ca.gov/toxics/id/taclist.htm](http://www.arb.ca.gov/toxics/id/taclist.htm)

California maintains a list of Toxic Air Contaminants (TACs) and a program for adding additional TACs.

## **B. Chemical Toxicity Data**

### **Ecological Structure Activity Relationships (ECOSAR)**

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

ECOSAR 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

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Structure Activity Relationships (SARs). The program estimates a chemical's acute (short-term) toxicity and, when available, chronic (long-term or delayed) toxicity.

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#### **Ecotox database**

<http://cfpub.epa.gov/ecotox/>

The Ecotox database provides single chemical toxicity information for aquatic and terrestrial life. This is a useful tool for evaluating the impact of chemicals on the environment.

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#### **EPA Triage Database**

[http://www.epa.gov/Se\\_triag/](http://www.epa.gov/Se_triag/)

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

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#### **Integrated Risk Information System (IRIS) Database**

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

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.

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#### **Toxic Substances Control Act Test Submissions (TSCATS)**

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

TSCATS 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 US 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 For Your Information (FYI) notice.

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#### **High Production Volume Information System (HPVIS)**

[www.epa.gov/hpvis/index.html](http://www.epa.gov/hpvis/index.html)

HPVIS provides complete and easy access to technical health and environmental effect information on chemicals that are manufactured or imported to US in volumes greater than 1MM lbs per year. Information in this database are submitted through HPV Challenge Program. HPVIS allows users to search for summary information, test plans, and new data on

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high production volume chemicals as they are developed.

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### **Chemical Fact Sheets**

[www.epa.gov/chemfact/](http://www.epa.gov/chemfact/)

The EPA's Office of Pollution Prevention and Toxics developed Chemical Fact to summarize information on a particular chemical including exposure, environment and human health hazard, environmental fate, regulatory information, and whom to contact for additional information.

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### **TOXNET**

[toxnet.nlm.nih.gov/](http://toxnet.nlm.nih.gov/)

TOXNET is a series of databases on chemical toxicity hosted by the National Institutes of Medicine, which allows multiple searching options. The databases include: ChemIDplus, HSDB, Toxline, CCRIS, DART, GENETOX, IRIS, ITER, LactMed, Multi-Database, TRI, Haz-Map, Household Products and TOXMAP.

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### **Enhanced ToxSeek Meta-Search Engine and Clustering Tool**

[toxseek.nlm.nih.gov](http://toxseek.nlm.nih.gov)

ToxSeek is an NLM metasearch engine and clustering tool that enables the simultaneous searching of many different toxicology and environmental health information databases and web sites. This tool includes 59 databases including the TOXNET Search tool, as well as information sources from NLM, NIH, US Government, International and other sources.

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### **Library of Chemical Information**

[www.cfsan.fda.gov/dms/chemist.html](http://www.cfsan.fda.gov/dms/chemist.html)

The Library of Chemical Information is maintained by the US Food and Drug Administration's Center for Food Safety and Applied Nutrition and is an excellent database for multiple classes of chemicals including food additives, cosmetics, color additives, pesticides and other chemicals.

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### **Fragrance or Flavor Components Database**

[rifm.org/nd/Login.cfm](http://rifm.org/nd/Login.cfm)

The Research Institute on Fragrance Materials maintains the most comprehensive world- wide source database on fragrance/flavor components including acute aquatic toxicity, biodegradation data, human health issues, for example, carcinogenesis, sensitization. A

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password is required to access the database.

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### **The Scorecard Database**

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

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

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### **International Chemical Safety Cards (ICSCs)**

<http://www.cdc.gov/niosh/ipcs/icstart.html>

ICSCs are made available by the National Institute for Occupational Safety and Health. They summarize safety information in 8 languages and indexed in a variety of ways.

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### **CleanGredients**

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

CleanGredients™ is an online database of cleaning product ingredients 'A one stop shop for green formulation'. The database contains physical chemical data, MSDS datasheets, and environmental and human health hazard data on raw materials used to formulate cleaning products.

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### **PubMed® MEDLINE®**

[www.pubmed.gov](http://www.pubmed.gov)

MEDLINE contains bibliographic citations and author abstracts from more than 5000 biomedical journals published in the United States and 80 other countries. The database includes over 15 million citations dating back to the mid-1950s.

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### **Managerial Technologies Corp (MTC) Safety Library**

[www.mtclibraries.com/lib/resource\\_locate.php?id=sl26949](http://www.mtclibraries.com/lib/resource_locate.php?id=sl26949)

The safety professional's online library, covering topics related to safety, safety ergonomics, fleet and environment. The Safety Library contains over 40 environmental databases and over 70 databases of chemical profiles. Subscription is required.

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### **Chemistry Links for Chemists**

[www.liv.ac.uk/Chemistry/Links/refdatabases.html](http://www.liv.ac.uk/Chemistry/Links/refdatabases.html)

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This website contains a list of 105 different databases from US and around the world.

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### **Environmental Health and Safety Freeware**

[www.ehsfreeware.com/cheminfo.htm](http://www.ehsfreeware.com/cheminfo.htm)

This website contains a list of almost 100 different EH&S databases that are all free plus several commercial databases.

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### **Arie/TM WebInsight**

[www.3ecompany.com/ariel\\_webinsight.com](http://www.3ecompany.com/ariel_webinsight.com)

Ariel™ Webinsight is a subscription-based online compliance management tool with an easy-to-use interface and robust search, query, reporting and analysis features. The tool provides access to current, accurate, comprehensive global regulatory content containing more than 700 searchable regulatory lists covering more than 75 countries; full-text repositories of legislation, international transportation data, as well as chemical property and hazard data.

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### **Infochems database**

[www.infochems.com/main/default.asp](http://www.infochems.com/main/default.asp)

Commercial service that provides chemical information for US and Global regulations. Contains chemical, physical and toxicity information. The database includes generic chemical names and commercial chemical names.

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### **American Conference of Governmental Industrial Hygienists (ACGIH)**

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

ACGIH maintains annual editions of the TLVs® and BEIs® which are used worldwide as a guide for evaluation and control of workplace exposures to chemical substances and physical agents. Threshold Limit Value (TLV®) occupational exposure guidelines are recommended for more than 700 chemical substances and physical agents. There are more than 50 Biological Exposure Indices (BEIs®) that cover more than 80 chemical substances.

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### **The Canadian Centre for Occupational Health and Safety (CCOHS's Databases)**

[ccinfoweb.ccohs.ca /](http://ccinfoweb.ccohs.ca/)

CCOHS's Web Information, a paid service, provides simple, one-step searching across many database collections

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### **CrossFire Beilstein**

[www.mdl.com/products/knowledge/crossfire\\_beilstein/](http://www.mdl.com/products/knowledge/crossfire_beilstein/)

The Crossfire Beilstein database is the world's largest compilation of chemical facts. This database indexes three primary data domains: substances, reactions and literature. The substance domain stores structural information with all associated facts and literature references, including chemical, physical and bioactivity data. The reaction domain details the preparation of substances, enabling scientists to investigate specific reaction pathways with reaction search queries.

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### **European Chemical Substances Information System (ESIS)**

[ecb.jre.it/esis/](http://ecb.jre.it/esis/)

ESIS is an IT system which provides you with information on chemicals

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### **eChemPortal**

[webnet3.oecd.org/eChemPortal/Home.aspx](http://webnet3.oecd.org/eChemPortal/Home.aspx)

The eChemPortal is an effort of the Organization for Economic Cooperation and Development (OECD) in collaboration with the European Commission, the United States, Canada, Japan, the International Council of Chemical Associations, the Business and Industry Advisory Committee, the World Health Organization's International Program on Chemicals and Chemical Safety, the United Nations Environment Program on Chemicals and non-governmental organizations.

eChemPortal offers free public access to information on properties and effects of chemical substances. It is an integrated system that allows users to simultaneously search multiple databases prepared for government chemical and review programs around the world.

The current version of eChemPortal offers the possibility to retrieve information by searching on chemical names or CAS Registry numbers. The second phase will incorporate additional search options to retrieve and compile specific hazard or other effects data (e.g., toxicity endpoints) from the participating databases.

At this time, the following databases participate in eChemPortal™\* European Chemical Substances Information System (ESIS, European Commission ), \*CHRIP (Japan's Information on Biodegradation and Bioconcentration of the Existing Chemical Substances in the Chemical Risk information platform), \*OECD HPV Database (OECD), \*Screening Information Datasets for High Volume Production Chemicals (UNEP Chemicals), \*HPVIS (US Environmental Protection Agency), \*INCHEM (IPCS).

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## **C. Exposure Assessment Tools**

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### **Environmental Fate Database (EFDB)**

[www.syrres.com/eSc/efdb.htm](http://www.syrres.com/eSc/efdb.htm)

EFDB has been developed in support of US EPA. It is comprised of DATALOG and BIOLOG, which contain environmental fate, microbial toxicity and biodegradation data.

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### **EPA's Environmental Fate Database for actives**

[cfpub.epa.gov/pfate/home.cfm](http://cfpub.epa.gov/pfate/home.cfm)

This database includes information on the environmental fate of pesticide actives.

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### **EPA's OPPT Exposure Assessment Tools and Models**

[www.epa.gov/opptintr/exposure/index.htm](http://www.epa.gov/opptintr/exposure/index.htm)

The Office of Pollution Prevention and Toxics (OPPT) has developed a series of methods, databases, and predictive models to help in evaluating what happens to chemicals when they are used and released into the environment. These tools are intended to be used by scientists and engineers familiar with exposure assessment principles.

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### **Greatest Potential for Human Exposure report**

[http://www.hc-sc.gc.ca/ewh-semtipubs/contaminants/existsublexposure/index\\_e.html](http://www.hc-sc.gc.ca/ewh-semtipubs/contaminants/existsublexposure/index_e.html)

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).

### **D. Hazard and Risk Assessment Tools**

International Uniform Chemical Information Database  
[ecb.jrc.it/iuclidS /](http://ecb.jrc.it/iuclidS/)

IUCLIDS is a software tool for entering and storing information on chemicals, as well as preparing and submitting dossiers to fulfil legislation requirement. For EU Chemicals Agency and Member States, it is the central data repository for all dossiers submitted, the basis for evaluating the risks of substances and requiring new information and for the basis for restricting and authorizing the use of chemicals to manage risks.

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### **Massachusetts Toxics Use Reduction Institute Pollution Prevention Options Analysis Tool**

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(p2oasys)

[www.turi.org/content/content/view/full/1125/](http://www.turi.org/content/content/view/full/1125/)

The Institute has developed P20aSys to help companies determine whether the Toxic Use Reduction (TUR) options they are considering may have unforeseen, negative environmental, worker or public health impacts. P20ASys allows companies to assess the 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.

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### **Report on the Advisory List for Self-Classification of Dangerous Substances**

[www.mst.dk/homepage/default.asp?Sub=http://www.mst.dk/udgiv/publications/2004/87-614-477-1/html/default\\_eng.htm](http://www.mst.dk/homepage/default.asp?Sub=http://www.mst.dk/udgiv/publications/2004/87-614-477-1/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 mean of QSAR models (Quantitative Structure-Activity Relationship) as having acute oral toxicity, mutagenicity, carcinogenicity, and/or danger to the aquatic environment.

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## **F. Safer Chemistry Design Tools**

### **Sustainable Futures Program (SF)**

[www.epa.gov/oppt/newchems/pubs/sustainablefutures.htm](http://www.epa.gov/oppt/newchems/pubs/sustainablefutures.htm)

The SF program is an approach that encourages pollution prevention in new chemical development through the transfer of OPPT's chemical risk screening methodologies.

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### **The Green Chemistry Expert System (CCES)**

[www.epa.gov/opptintr/greenchemistry/tools.html](http://www.epa.gov/opptintr/greenchemistry/tools.html)

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. The GCES features are contained in five modules:

- Synthetic Methodology Assessment for Reduction Techniques (SMART)
  - Green Synthetic Reactions
  - Designing Safer Chemicals
  - Green Solvents/Reaction Conditions
  - Green Chemistry References.
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### **The Green Screen for Safer Chemicals**

[www.cleanproduction.org/Green.Greenscreen.php](http://www.cleanproduction.org/Green.Greenscreen.php)

The Green Screen for Safer Chemicals is a method for assessing and benchmarking chemical alternatives based on their hazard characteristics developed by Clean Production Action. The Green Screen builds on new chemicals assessment protocols developed by the USEPA and adapted for comparing alternatives by the USEPA Design for the Environment Program. It identifies chemical characteristics of high concern and characteristics of increasingly greener chemicals.

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### **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.

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### **Swedish Chemicals Inspectorate PRIO Program**

[www.kemi.se/templates/PRIOEngframes\\_4144.aspx](http://www.kemi.se/templates/PRIOEngframes_4144.aspx)

PRIO is a web-based tool intended to be used to preventively reduce risks to human health and the environment from chemicals. 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.

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### **Control of Substances Hazardous to Health Regulations (COSHH)**

[www.coshh-essentials.org.uk/](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, for example, mixing or drying.

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### **Safer Solvent Alternatives**

[www.irta.us](http://www.irta.us)