

The Tools for HPV Chemical Assessment & Safer Design

Green Chemistry in Commerce Council

Session 6A

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DC Long
12/14/06

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Why is a Tools Database Needed

- Companies, Universities and other chemical users have difficulty finding meaningful chemical information to safely use, work with and dispose of chemicals.
- MSDS are required by OSHA but they often provide minimal information. They often lack information to understand the toxicity, long term hazards, environmental fate, properties or even the composition.
- Information on many chemicals or modeling tools exist but can be difficult to locate

Tools Database Goals

- Provide a single location that provides multiple resources for chemical properties, toxicity and environmental data.
- Provide links for each resource. The link may need updated rather than recreating a database where information needs to be updated periodically.
- Provide user comments describing the database or modeling programs. Can include comments on ease of use and validity of the information. Describe limitations to the database or modeling program. Comments can be added by users over time.

What Tools & Databases are Available

- There are numerous free sources of chemical data. One must search to find the databases.
- There are also several excellent subscriber chemical databases.
- In addition to databases there are numerous chemical modeling programs for hazard and risk assessment, exposure assessment tools, fate assessment tools and safer chemistry design tools

GC3 Tools Database

Lets take a look at the current organization of the database

Environmental/Chemical Properties

Chemical Properties/Toxicity/Safety

Chronic Toxicity

Multiple Databases (including subscriber)

Modeling Programs- Assessment Tools

Environmental and Chemical Properties

Copy of Chemistry tools12-04-06.xls					
Environmental/Chemical Properties					
Database	URL	Source	Comment	Ease of Use	
Cefas Toxicity Database	http://www.cefas.co.uk/basic/toxdataP.htm	Cefas, UK	Chemicals listed by name. Has toxicity standards by country, UK, EC, US, Can. Other.	E	
Ecotox Database	http://cfpub.epa.gov/ecotox/	US EPA Office of Solid Waste and Emergency Response	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	E	
ARS Pesticide Properties Database	http://www.arsusda.gov/acsl/services/ppdb/listall.html	USDA	Includes 334 widely used pesticides. Information focuses on the 16 most important properties that affect pesticide transport and degradation. Last updated in 1995. Data is over 10 years old.	E	
8(e) Triage Chemical Studies Database	http://www.epa.gov/8e_triage/	US EPA Office of OPPT	Searchable database of scientific studies on health and environmental effects of toxic chemicals related to section 8(e) of TSCA. Must install a program to search the database.	M	
Environmental Fate Database	http://www.syrres.com/esc/efdb.htm	Syracuse Research Corp	Has been developed in support of US EPA. It comprises of a DATALOG and BIOLOG which contains environmental fate, microbial toxicit and biodegradation data. This is a good database.	E	
EPA's Envir. Fate Database for actives	http://cfpub.epa.gov/pfate/home	US EPA	Database which includes the environmental fate of pesticide actives	M	
Fragrance or Flavor Components Database	http://rifm.org/nd/Login.cfm	RIFM/FEMA	Envir. Info incl. Fish LC50s, biodegradation data. Human health issues, e.g. carcinogenesis, sensitization. Must have password	NA	

Environmental Fate Database

- Environmental Science
- estimation software
- databases
- expert consulting
- toxicology & risk assessment
- environmental chemistry
- free demos & databases
 - EFDB
 - TSCATS
 - KOW
 - ozone depletion/global warming
 - PHYSPROP
 - ISE model
- reports/presentations
- research publications
- research investigations
 - of interest
 - related links
 - guest book
- PRA Center of CNY
- Upstate NY SRA

Business Areas

environmental science

..... free demos & databases



Environmental Fate Data Base (EFDB)

Substructure search all of EFDB, TSCATS and PHYSPROP using [Chems³](#).

Click on one of the buttons below to search the database online.
Click here for [more information](#).

DATALOG

DATALOG is a bibliographic file containing 18 types of environmental fate data.

BIOLOG

BIOLOG, or the Microbial Degradation/Toxicity File, provides sources of microbial toxicity and biodegradation data.

CHEMFATE

CHEMFATE is a data value file containing 25 categories of environmental fate and physical/chemical property information on commercially important chemical compounds.

BIODEG

BIODEG contains experimental values relating to biodegradation subjects.

BIODEG SUMMARY provides summary information and

Chemical Properties/Toxicity/Safety

Microsoft Excel

File Edit View Insert Format Tools Data Window Help Adobe PDF

Type a question for

D22 Good search for many chemicals, acute toxicity and chemical/physical characteristics.

Copy of Chemistry tools12-04-06.xls

	A	B	C	D	E	F
15	Chemical Properties/Toxicity/Safety					
16	Database	URL	Source	Comment	Ease of Use	
17	Household Products Database	http://householdproducts.nlm.nih.gov/	US Library of Medicine	Contains information on common products used in the home. Provides ingredient, health effects and safety data on thousands of products. Is not always up to date.	E	
18	HPV Challenge Program Chemical List	http://www.epa.gov/chemrtk/pubs/update/hpvchmlt.htm	US EPA Office of OPPT	Contains about 2,800 chemicals that have been manufactured or imported to US in volumes greater than 1MM lbs per year. Limited number of chemicals and data available.	E	
19	Library of Chemical Information	http://www.cfsan.fda.gov/~dms/chemist.html	USDA	Excellent database for multiple classes of chemicals including food additives, cosmetics, color additives, pesticides and other chemicals	E	
20	Master Summary for the Chemical Hazard Data	www.epa.gov/chemrtk/pubs/general/hazchem.htm	US EPA Office of OPPT	Contains information of whether or not data on six hazard endpoints are publicly available for about 3000 HPV chemical, acute toxicity, chronic toxicity, teratogenicity, developmental and reproductive toxicity, mutagenicity, ecotoxicity and environmental fate.	E	
21	CleanGredients	http://www.cleangredients.org/	GreenBlue	Database of surfactants. Surfactant suppliers have provided chemical, physical, toxicological, and environmental data for a variety of surfactants. Database is searchable	E	
22	Chem ID	http://chem.sis.nlm.nih.gov/chem	National Library of Health	Good search for many chemicals, acute toxicity and	E	
23	WHO Water Quality Guidelines	http://www.who.int/water_sanitation_health/dwg/gdwg3/en/	World Health Organization	International standards for selected chemical, microbiology and other parameters.	E	
	International Chemical			Summarizes safety information in 8 languages and indexed in a variety of ways. Summarizes health		

Sheet1 / Sheet2 / Sheet3 /



High Production Volume (HPV) Challenge Program

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Chemical Hazard Data Availability Study

High Production Volume (HPV) Chemicals and SIDS Testing

Of the 3,000 chemicals that the US imports or produces at more than 1 million lbs/yr, a new EPA analysis finds that 43% of these high production volume chemicals have no testing data on basic toxicity and only seven percent have a full set of basic test data. This lack of test data compromises the public's right to know about the chemicals that are found in their environment, their homes, their workplace, and the products that they buy. Industry must do more to ensure that basic information is available on every high-production chemical they manufacture.

Background:

There are six basic tests which have been internationally agreed to for screening high production volume (HPV) chemicals for toxicity. The tests agreed to under the Organization for Economic Cooperation and Development's Screening Information Data Set (OECD/SIDS) program are: acute toxicity; chronic toxicity; developmental/reproductive toxicity; mutagenicity; ecotoxicity and environmental fate.

EPA found that approximately 55% of TRI chemicals have had full SIDS testing, while only 7% of other chemicals have full test data. EPA also looked at a set of 491 chemicals used by children and families in consumer products. Only 25% of these chemicals have full screening data. EPA cannot begin to judge the hazards and risks of such consumer chemicals without basic information, and in fact substantially more detailed and exhaustive testing is needed to assess these high exposure chemicals.

It is clear that companies need to do more to address this problem: of the 830 companies making HPV chemicals in the US, 148 companies have NO SIDS data available on their chemicals; an additional 459 companies sell products for which, on average, half or less of SIDS tests are available. Only 21 companies (or 3% of the 830 companies) have all SIDS tests available for their chemicals. The basic set of test data costs about \$200,000 per chemical.

EPA's Plans:

How to Participate
Who's Participating
Information on HPV Chemicals
HPV Challenge Program Robust Summaries, Test Plans & Comments
Children's Chemical Eval. Pgm.
Related Websites



HPV Challenge Program

U.S. Environmental Protection Agency

High Production Volume (HPV) Challenge Program

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- How to Participate
- Who's Participating
- Information on HPV Chemicals
- HPV Challenge Program Robust Summaries, Test Plans & Comments
- Vol. Children's Chemical Eval. Pgm.
- Related Websites

Search the HPV Chemical List

By using the drop-down menus, you can search the 1990 or 1994 list by CAS Number, Chemical Name, Indicator value, Chemical Sponsorship Status, or Sponsor Commitment Status. You can enter all or part of a CAS number or chemical name, a single indicator value, a single chemical sponsorship value, sponsor name, or sponsorship year.

Please note that dashes have been added to all CAS Numbers on this website. This change ensures that all CAS Numbers conform to standard CAS format. Dashes must now be included when searching for a CAS Number.

Search Type -

Search Term-

Search Year-

Indicator Column Values

0 = Chemical is within the scope of the HPV Challenge Program and may be sponsored.

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1 of 33

Internet

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RECEIVED
OPPT CBIC

HPV 201-16155

DATA SUMMARY AND TEST PLAN

FOR

PHENOL, 4,4'-ISOPROPYLIDENBIS[2,6-DIBROMO-

(TETRABROMOBISPHENOL A, TBBPA)

CAS No. 79-94-7

Select Text Tool

114%

Save a Copy Print Email Search Review & Comment Sign

http://www.epa.gov/HPV/pubs/summaries/phenolis/c13460rt3.pdf

Edit View Favorites Tools Help

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Chronic Toxicity Database

of Chemistry tools12-04-06.xls					
A	B	C	D	E	F
Chronic Toxicity Database					Ease of Use
Database	URL	Source	Comment	Ease of Use	
Proposition 65	http://www.oehha.ca.gov/prop65.html	California Office of Health Hazard Assessment	List of chemicals that have been confirmed to be carcinogens and or reproductive toxins. Chemicals are listed by name and by CAS #	E	
Integrated Risk Information System (IRIS)	http://www.epa.gov/iris/	US EPA Office of OPPT	This is a data base that summarizes the health effects of exposure to chemicals. It is intended to be used without extensive training but user should have some knowledge of health science.	E	
National Toxicology Program Report on Carcinogens	http://ntp.niehs.nih.gov/ntp/roc/toc11.html	National Institute of Health	Listing of chemicals that are carcinogen, likely carcinogens or probable carcinogens.	E	
Chronic Toxicity Database	http://www.leadscope.com/fdad_b_cat.php	FDA	High quality genetic toxicity database from the US FDA CFSAN (Center for Food Safety and Applied Nutrition). Includes 484 chemical structures and 4373 genetic toxicity studies on the following endpoints: bacterial mutagenesis, in vitro mammalian mutagenesis, in vitro mammalian chromosomal aberrations and in vivo mammalian micronuclei. High quality chronic toxicity database from the US FDA CDER. (Center for Drug Evaluation and Research). Chronic toxicity data from CDER including information on clinical signs, clinical pathology, clinical chemistry, hematology and histopathology. Data captured on rat and mouse for 1 year, 6 month and 3 month studies.	M	

adscope Home » FDA Toxicity Databases



FDA CFSAN 2006 Genetox Database*

\$250 [Add to Cart](#)

High quality genetic toxicity database from the US FDA CFSAN (Center for Food Safety and Applied Nutrition).

Includes 484 chemical structures and 4373 genetic toxicity studies on the following endpoints: bacterial mutagenesis, *in vitro* mammalian mutagenesis, *in vitro* mammalian chromosomal aberrations and *in vivo* mammalian micronuclei.

FDA CDER 2006 Genetox Database*

\$250 [Add to Cart](#)

High quality genetic toxicity database from the US FDA CDER (Center for Drug Evaluation and Research).

Genetic toxicity information extracted from pharmacological reviews contained in New Drug Approvals (NDA). Endpoints include: bacterial mutagenesis, *in vitro* mammalian mutagenesis, *in vitro* mammalian chromosomal aberrations and *in vivo* mammalian micronuclei.

FDA CDER 2006 Chronic/subchronic Database*

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High quality chronic toxicity database from the US FDA CDER (Center for Drug Evaluation and Research).

Chronic toxicity data from CDER including information on clinical signs, clinical pathology, clinical chemistry, hematology and histopathology. Data captured on rat and mouse for 1 year, 6 month and 3 month studies.

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Prop 65 Chemical Database

Welcome to *California*



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[Ecotoxicology](#)

[Education](#)

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[Pesticides](#)

[Proposition 65](#)

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[Risk Assessment](#)

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Proposition 65

Proposition 65, the [Safe Drinking Water and Toxic Enforcement Act of 1986](#), was enacted as a ballot initiative in November 1986. The Proposition was intended by its authors to protect California citizens and the State's drinking water sources from chemicals known to cause cancer, birth defects or other reproductive harm, and to inform citizens about exposures to such chemicals.

Proposition 65 requires the Governor to publish, at least annually, [a list of chemicals known to the state to cause cancer or reproductive toxicity](#).

Questions about Proposition 65? Check our [Frequently asked Questions](#) page or contact Cynthia Oshita or Susan Luong in the Proposition 65 office: (916)445-6900 or email Cynthia Oshita at coshita@oehha.ca.gov or email Susan Luong at sluong@oehha.ca.gov

 search

OEHHA My CA

Proposition 65 Links

What's New

- [Acrylamide](#)

[Current List of Chemicals](#)

[Safe Harbor Numbers \(HSRLs/MADLs\)](#)

[Calendar](#)

[General Background](#)

[Proposition 65 Frequently Asked Questions](#)

[Workshop/Meeting Materials](#)

[CRIIR Notices](#)

- [Changes to Prop 65 List](#)

Sources with Multiple Databases

Multiple Databases					
Data Base	URL	Source	Comment		
Chemical Fact Sheets	http://www.epa.gov/chemfact/	US EPA Office of OPPT	Chemical fact sheets and summaries in PDF format	E	
Chemical Backgrounders	http://www.nsc.org/library/chemical/index.htm	National Safety Council	Chemical descriptors including properties, health effects, exposure and regulatory information.	E	
EXTOXNET		U of CA, Davis, Oregon State, MI State, Cornell and U of Idaho	Various types of pesticide toxicological and environmental chemistry data	E	
Chemfinder	http://chemfinder.cambridgesoft.com/	Cambridgesoft Corp-	information about specific chemical with links to other websites with even more information. Easy to use. Fee for service	NA	
MTC Library	http://www.mtclibraries.com/lib/resource_locate.php?id=sl26949		Multiple databases and modeling programs. Subscription required	NA	
Chemistry Links for Chemists	http://www.liv.ac.uk/Chemistry/Links/refdatabases.html	Virtual Library	List of 105 different databases from US and around the world		
Environmental Health and Safety Freeware	http://www.ehsfreeware.com/cheminfo.htm		A list of almost 100 different EH&S databases that are all freeware plus several commercial databases. Good starting place to search for chemical information.	E	
Ariel Chemical database	http://www.3ecompany.com/EHS_MSDS_Solutions/ariel_regulatory.html?source=gadwords	3E Corp.	Commercial service that provides chemical information for US and Global regulations. Contains chemical, physical and toxicity information	NA	
Infochem database	http://www.infochems.com/main/default.asp	Infochems Inc.	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.	NA	

What the Libraries Offer	Hot Topics	 MTC Libraries <i>Managerial Technologies Corp Resource Libraries</i> The Business Library The HR Library rmLibrary The Safety Library The Healthcare Library The Transportation Library	Libraries Overview	Subscribe
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Site Map	Professional Guides		FAQ	Contact Us
Search the Library	Special Resources		Marketing Partner Programs	Library Main Entrance

MTC Libraries

Resource : ECOSAR Ecological Structure Activity Relationships [26949]

Estimate the toxicity of chemicals used in industry and discharged into water

Click on any of the MTC Libraries below to find this and similar resources:

Software : Environmental Software

Download software for EPA safety & health programs, site-specific sampling

Over 40 software programs on the environment. Environmental exposure assessment modeling software. Ecotox Thresholds calculations. Datasets and software programs for environmental professionals. Interactive system for selecting models (air, surface water, ground water and multimedia). AFR - Automated Form R - electronic form companies complete to report toxic chemicals released into land, water, or air. Oil spill tools. Soil Screening Calculations.

Environment : Software

Download software for EPA safety & health programs, site-specific sampling

Over 40 software programs on the environment. Environmental exposure assessment modeling software. Ecotox Thresholds calculations. Datasets and software programs for environmental professionals. Interactive system for selecting models (air, surface water, ground water and multimedia). AFR - Automated Form R - electronic form companies complete to report toxic chemicals released into land, water, or air. Oil spill tools. Soil Screening Calculations.

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Name=Struct		Search	About
NCI		Search	About Trial
The Merck Index		Search	About Trial
Ashgate Drugs		Search	About Trial

Chemical Databases

ChemACX Pro		Search	About Trial
ChemACX Pro & ChemACX-SC Pro	CD only		About

Reaction Databases

Organic Syntheses	FREE	Search	About
ChemReact500		Search	About Trial
ChemReact68		Search	About Trial



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Commercial Price: \$40.00
Educational Price: \$10.00



CHEMICAL INFORMATION

Following is a list of freeware that provides information on chemical properties and regulated chemicals. To learn more about a particular item, click on the item name. To download a software product or visit an interactive web site, click on "download" or "view," respectively. But first, please read our [disclaimer and permissions](#) page if you haven't already done so.

[3\(e\) Triage Chemical Studies Database](#)

By US Environmental Protection Agency, Office of Pollution Prevention and Toxics (OPPT). Searchable database of scientific studies on the health and environmental effects of toxic chemicals related to Section 8(e) of TSCA.
[download](#)

[ARS Pesticide Properties Database](#)

By US Department of Agriculture, Agricultural Research Service. A database of chemical and physical properties of 334 widely used pesticides. Information included in the database focuses on 16 of the most important properties that affect pesticide transport and degradation characteristics.
[visit](#)

[Atomic Weights and Isotopic Compositions](#)

By National Institute of Standards and Technology. The atomic weights are available for elements 1 through 111, and isotopic compositions or abundances are given when appropriate.
[visit](#)



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Modeling & Assessment Programs

Data Base	URL	Source	Comment		
PBT Profiler	http://www.pbtprofiler.net/	US EPA	Modeling program based on CAS # and chemical structure estimates the chemical's environmental persistence, bioaccumulation potential and toxicity. This is only an estimate and data can be used to confirm or exhaunerate as a PBT	M	
Ecological Structure Activity Relationships (ECOSAR)	http://www.epa.gov/oppt/newchems/tools/21ecosar.htm	US EPA Office of OPPT	Modeling program used to estimate the toxicity of chemical used in industry and discharged to water. Predicts toxicity to fish, invertebrates, algae using Structure Activity Relationships (SAR)	M	
Internet Geographical Exxposure Modeling System	http://www.epa.gov/opptintr/exposure/pubs/gems.htm	US EPA	Brings together in one system several EPA environmental fate and transport models and one of the environmental data need to run them	M	
Estimation Program Interface (EPI) Suite	http://www.epa.gov/opptintr/exposure/pubs/episuite.htm	US EPA	estimates physical/chemical properties and transport and includes estimation programs for LogKOW,KOC, atmospheric oxidation potential, Henry's law Constant, Water Solubility, melting Point, Vapor Pressure, Biodegradation, Bioconcentration Factor, Hydrolysis, Sewage Treatment Removal	E	
EFAST	http://www.epa.gov/opptintr/exposure/docs/efast.htm	US EPA	Exposure,Fate Assessment Screening Tool provides screening level estimates of concentrations of chemical released to air, surface water landfills, and from consumer products. Estimates potential inhalation, dermal and ingestion dose rate resulting from a release.	M	

Results

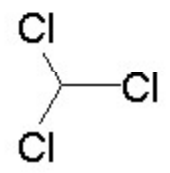
Orange or red highlights indicate that the EPA [criteria](#) have been exceeded.
[Black-and-white version](#)

[Persistence](#) [Bioaccumulation](#) [Toxicity](#)

67-66-3 Methane, trichloro-

PBT Profiler Estimate = PBT

Media	Half-Life (days)	Percent in Each Medium	BCF	Fish ChV (mg/l)
Water	38	43%	6.6	30
Soil	75	14%		
Sediment	340	0%		
Air	150	43%		



[P2 Considerations and more information](#)

The PBT Profiler Results are available for 20 minutes

EOCSAR

U.S. Environmental Protection Agency



New Chemicals Program

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EPA Home > Prevention, Pesticides & Toxic Substances > Pollution, Prevention & Toxics > New Chemicals Program > ECOSAR

Ecological Structure Activity Relationships



v. 0.99g, January, 2000

What is ECOSAR?

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.

What is a Structure Activity Relationship (SAR)?

Structure Activity Relationships, or SAR, is a technique routinely used by EPA to estimate aquatic toxicity of chemicals being reviewed by the EPA in response to Pre-Manufacture Notices mandated by Section 5 of the Toxic Substances Control Act (TSCA). ECOSAR makes EPA's SAR methods for aquatic toxicity conveniently available through an easy-to-use computer program.

How Does ECOSAR Work?

ECOSAR uses SARs to predict the aquatic toxicity of chemicals based on their structural similarity to chemicals for which aquatic toxicity data is available. SARs express the correlations between a compound's physicochemical properties and its aquatic toxicity. SARs measured for one compound can be used to predict the toxicity of similar compounds belonging to the same chemical class. ECOSAR also allows access to over 100 SARs developed for 42 chemical classes. The SARs contained within the program are based on test data. Many of the SAR predictions have been validated.

- Chemicals
- Forms and Information
- Manufacture Notice Status
- Chemicals Policies
- Advanced Materials
- Chemical Categories Report
- Send Orders and Significant New Use Fees
- SAR: Ecological Structure Activity Relationships
- Reporting and Reporting New Chemicals

Summary

- GC3 Spreadsheet of Chemical Information Databases and Modeling programs is just a start.
- It is currently a spreadsheet but could be transferred to a database like Access that is searchable using Key Words.
- GC3 Members need to use the tool to evaluate how useful it is and is it worth developing further.
- The GC3 Tools Team will be evaluating the tool and making recommendations. We invite others to provide input based on this presentation.