

# The Tools for HPV Chemical Assessment & Safer Design

Green Chemistry in Commerce Council

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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 rather than recreate a database where information needs to be updated periodically.
- Provide user comments describing the database or modeling programs. Include comments on ease of use and validity of the information. Describe limitations to the database or modeling program.

# 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 draft of the database

Current Organization:

Environmental/Chemical Properties

Chemical Properties/Toxicity/Safety


Chronic Toxicity

Multiple Databases (including subscriber)

Modeling Programs- Assessment Tools

# Environmental and Chemical Properties

Environmental/Chemical Properties				
Database	URL	Source	Comment	Ease of Use
Cefas Toxicity Database	<a href="http://www.cefas.co.uk/basic/toxdataP.htm">http://www.cefas.co.uk/basic/toxdataP.htm</a>	Cefas, UK	Chemicals listed by name. Has toxicity standards by country, UK, EC, US, Can. Other.	E
Ecotox Database	<a href="http://cfpub.epa.gov/ecotox/">http://cfpub.epa.gov/ecotox/</a>	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	<a href="http://www.arsusda.gov/acsl/services/ppdb/listall.html">http://www.arsusda.gov/acsl/services/ppdb/listall.html</a>	USDA	includes 334 widely used pesticides. Information focuses on the 16 most important properties that affect pesticide transport and degradation. Last updated in 1995	E
8(e) Triage Chemical Studies Database	<a href="http://www.epa.gov/8e_triag/">http://www.epa.gov/8e_triag/</a>	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.	E
Environmental Fate Database	<a href="http://www.syrres.com/esc/efdb.htm">http://www.syrres.com/esc/efdb.htm</a>	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	<a href="http://cfpub.epa.gov/pfate/home">http://cfpub.epa.gov/pfate/home</a>	US EPA	Database which includes the environmental fate of pesticide actives	M
Fragrance or Flavor Components Database	<a href="http://rifm.org/nd/Login.cfm">http://rifm.org/nd/Login.cfm</a>	RIFM/FEMA	Envir. Info incl. Fish LC50s, biodegradation data. Human health issues, e.g. carcinogenesis, sensitization. Must have password .....	NA

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# 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 [ChemS<sup>3</sup>](#).

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.



# Search for Ethanol Amine

## DATALOG Search Parameters

CAS#: 000141-43-5

Formula: C2H7NO

Name: ETHANOLAMINE

Print full reference list  Yes  No

Only references published since 1900

*Limit Search by selecting data types listed below.*

*NO SELECTIONS will cause ALL records for chemical to be retrieved.*

Number of records present for each data type is indicated next to the data type name.

- |  |  |
|--|--|
| <input type="checkbox"/> 1 ADSORP - Adsorption                 | <input type="checkbox"/> 1 HENRY CON - Henry's Law Constant          |
| <input type="checkbox"/> 2 BIOCON - Bioconcentration           | <input type="checkbox"/> 0 HYDROL - Hydrolysis                       |
| <input type="checkbox"/> 6 BIODEG - Biodegradation             | <input type="checkbox"/> 5 MONIT - Monitoring                        |
| <input type="checkbox"/> 7 DISS CON - Dissociation Constant    | <input type="checkbox"/> 5 OCCUP - Occupational Concentrations       |
| <input type="checkbox"/> 0 ECOS - Ecosystems                   | <input type="checkbox"/> 3 O/W PART - Octanol/Water Partition Coeff. |
| <input type="checkbox"/> 2 EFFL - Effluent Concentrations      | <input type="checkbox"/> 3 PHOTOOXID - Photooxidation                |
| <input type="checkbox"/> 0 EVAW - Evaporation from Water       | <input type="checkbox"/> 0 UV - UV Spectra                           |
| <input type="checkbox"/> 2 FOOD - Food and Crop Concentrations | <input type="checkbox"/> 14 VP - Vapor Pressure                      |
| <input type="checkbox"/> 0 FIELD - Field Studies               | <input type="checkbox"/> 10 WATER SOL - Water Solubility             |

Begin search

Reset Values

# Chemical Properties/Toxicity/Safety

Chemical Properties/Toxicity/Safety				
Database	URL	Source	Comment	Ease of Use
Household Products Database	<a href="http://householdproducts.nlm.nih.gov/">http://householdproducts.nlm.nih.gov/</a>	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
HPV Challenge Program Chemical List	<a href="http://www.epa.gov/chemrtk/pubs/update/hpvchmlt.htm">http://www.epa.gov/chemrtk/pubs/update/hpvchmlt.htm</a>	US EPA Office of OPPT	Contains about 2,800 chemical that have been manufactured or imported to US in volumes greater than 1MM lbs per year. Limited number of chemicals and data available.	E
Library of Chemical Information	<a href="http://www.cfsan.fda.gov/~dms/chemist.html">http://www.cfsan.fda.gov/~dms/chemist.html</a>	USDA	Excellent database for multiple classes of chemicals including food additives, cosmetics, color additives, pesticides and other chemicals	E
Master Summary for the Chemical Hazard Data	<a href="http://www.epa.gov/chemrtk/pubs/general/hazchem.htm">www.epa.gov/chemrtk/pubs/general/hazchem.htm</a>	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
CleanGredients	<a href="http://www.cleangredients.org/">http://www.cleangredients.org/</a>	GreenBlue	Database of surfactants. Surfactant suppliers have provided chemical, physical, toxicological, and environmental data for a variety of surfactants. Database is searchable	E
Chem ID	<a href="http://chem.sis.nlm.nih.gov/chem">http://chem.sis.nlm.nih.gov/chem</a>	National Library of Health	Good search for many chemical, acute toxicity and chemical/physical characteristics.	E
WHO Water Quality Guidelines	<a href="http://www.who.int/water_sanitation_health/dwg/gdwq3/en/">http://www.who.int/water_sanitation_health/dwg/gdwq3/en/</a>	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	

# Households Products Database

## Household Products Database

National Institutes of Health  
National Library of Medicine  
Specialized Information Services



Home

Products

Ingredients

MSDS

Quick Search

### Browse & Search

- [Products](#)
- [Ingredients](#)
- [Material Safety Data Sheet \(MSDS\)](#)

### Support Pages

- [About](#)
- [FAQ](#)
- [Help](#)
- [Glossary](#)
- [Contact Us](#)
  
- [Other Resources](#)

### Health & Safety Information on Household Products

What's under your kitchen sink, in your garage, in your bathroom, and on the shelves in your laundry room? Learn more about what's in these products, about potential health effects, and about safety and handling.

Information in the Household Products Database is taken from a variety of publicly available sources, including brand-specific labels and Material Safety Data Sheets (MSDS) prepared by manufacturers.

### [Find a product...](#)

For advice if someone is poisoned, call your local [Poison Center](#) at (1-800-222-1222).



# 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  
I. Children's Chemical Eval. Pgm.  
Related Websites



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**HPV**

**201-16155**

**DATA SUMMARY AND TEST PLAN**

**FOR**

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

**(TETRABROMOBISPHENOL A, TBBPA)**

**CAS No. 79-94-7**



# CleanGredients

for I&I Cleaning Products

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Welcome to the home of CleanGredients™, the online resource for green formulation.

### › Request for Comments on Attributes and Criteria for Solvents

We are developing the next CleanGredients™ module for solvents and seek your input on the relevant attributes and criteria to include. Please visit the "Request for Comments: CleanGredients™ Solvents" survey at: <http://www.surveymonkey.com/s.asp?u=660612411614> to submit your recommendations. If you or anyone else from your organization is interested in serving on a Technical Advisory Committee – for solvents or other ingredient classes, please [contact us](#).

The first meeting of the solvent TAC will be held on December 11 at 3pm EASTERN. Please let us know if you plan to participate.

### › CleanGredients™ for surfactants is here!

GreenBlue is now accepting surfactant listings and CleanGredients™ [memberships](#) for formulators and suppliers. The first 100 ISSA members to subscribe to CleanGredients™ receive a 20% discount. Credit card payments can now be accepted by telephone.

# Chronic Toxicity Databases

Chronic Toxicity					
Database	URL	Source	Comment	Ease of Use	
CA Proposition 65	<a href="http://www.oehha.ca.gov/prop65.html">http://www.oehha.ca.gov/prop65.html</a>	California Office of Health Hazard Assessment	List of chemical 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)	<a href="http://www.epa.gov/iris/">http://www.epa.gov/iris/</a>	US EPA Office of OPPT	This is a data base that summarizes the health effects of exposure to chemical. 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	<a href="http://ntp.niehs.nih.gov/ntp/roc/toc11.html">http://ntp.niehs.nih.gov/ntp/roc/toc11.html</a>	National Institute of Health	Listing of chemicals that are carcinogen, likely carcinogens or probable carcinogens.	E	
FDA Toxicity Database	<a href="http://www.leadscope.com/fdadb_cat.php">http://www.leadscope.com/fdadb_cat.php</a>	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	

Leadscope 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\*

\$250 [Add to Cart](#)

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.

#### Shopping Cart

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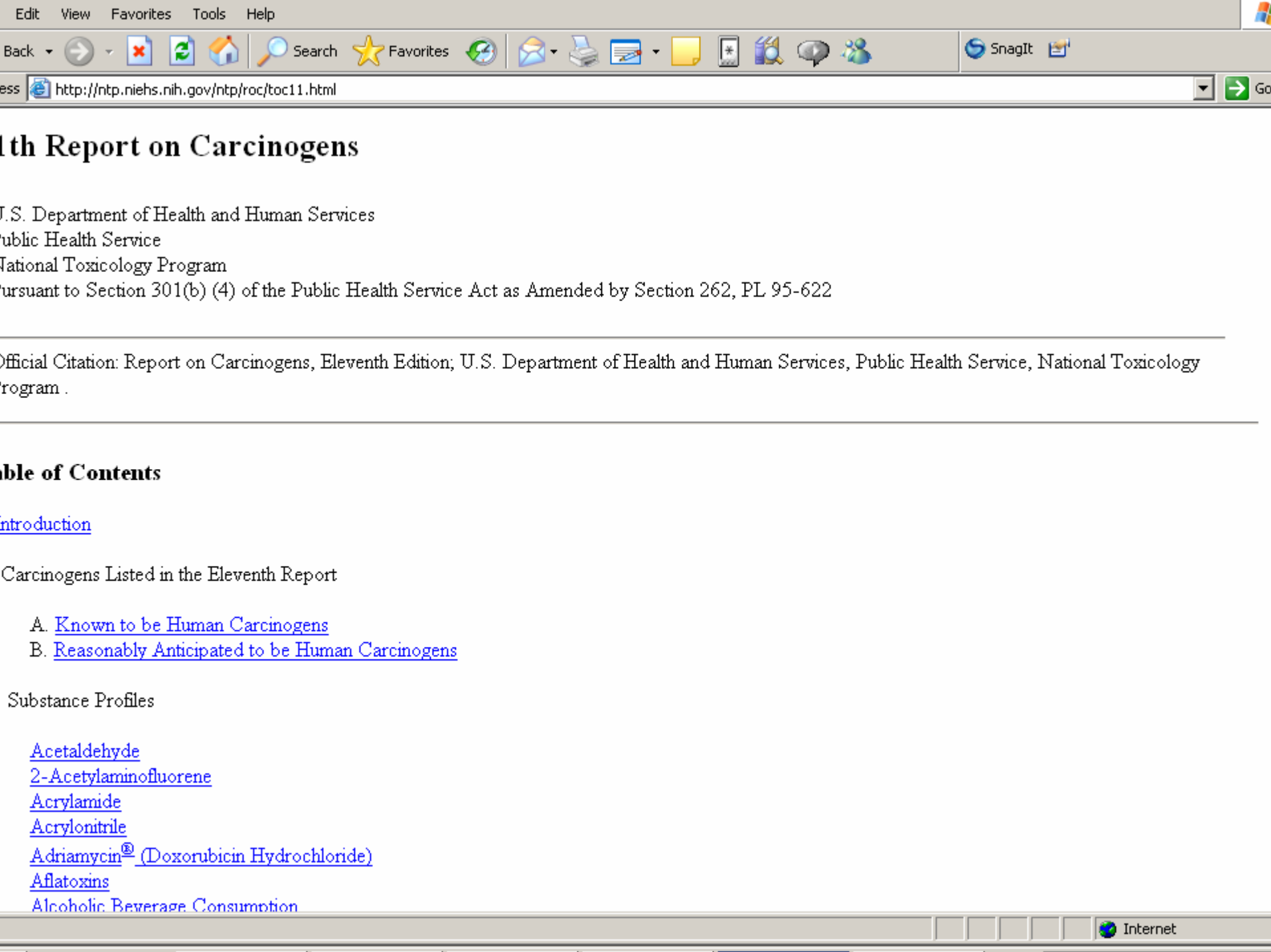
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# Eleventh Report on Carcinogens

U.S. Department of Health and Human Services

Public Health Service

National Toxicology Program

Pursuant to Section 301(b) (4) of the Public Health Service Act as Amended by Section 262, PL 95-622

Official Citation: Report on Carcinogens, Eleventh Edition; U.S. Department of Health and Human Services, Public Health Service, National Toxicology Program .

## Table of Contents

[Introduction](#)

Carcinogens Listed in the Eleventh Report

- A. [Known to be Human Carcinogens](#)
- B. [Reasonably Anticipated to be Human Carcinogens](#)

Substance Profiles

[Acetaldehyde](#)

[2-Acetylaminofluorene](#)

[Acrylamide](#)

[Acrylonitrile](#)

[Adriamycin<sup>®</sup> \(Doxorubicin Hydrochloride\)](#)

[Aflatoxins](#)

[Alcoholic Beverage Consumption](#)

# Sources with Multiple Databases

Data Base	URL	Source	Comment		
Chemical Fact Sheets	<a href="http://www.epa.gov/chemfact/">http://www.epa.gov/chemfact/</a>	US EPA Office of OPPT	Chemical fact sheets and summaries in PDF format	E	
Chemical Backgrounders	<a href="http://www.nsc.org/library/chemical/index.htm">http://www.nsc.org/library/chemical/index.htm</a>	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	<a href="http://chemfinder.cambridgesoft.com/">http://chemfinder.cambridgesoft.com/</a>	Cambridgesoft Corp-	information about specific chemical with links to other websites with even more information. Easy to use. Fee for service	NA	
MTC Library	<a href="http://www.mtclibraries.com/lib/resource_locate.php?id=sl26949">http://www.mtclibraries.com/lib/resource_locate.php?id=sl26949</a>		Multiple databases and modeling programs. Subscription required	NA	
Chemistry Links for Chemists	<a href="http://www.liv.ac.uk/Chemistry/Links/refdatabases.html">http://www.liv.ac.uk/Chemistry/Links/refdatabases.html</a>	Virtual Library	List of 105 different databases from US and around the world		
Environmental Health and Safety Freeware	<a href="http://www.ehsfreeware.com/cheminfo.htm">http://www.ehsfreeware.com/cheminfo.htm</a>		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	<a href="http://www.3ecompany.com/EHS_MSDS_Solutions/ariel_regulatory.html?source=gadwords">http://www.3ecompany.com/EHS_MSDS_Solutions/ariel_regulatory.html?source=gadwords</a>	3E Corp.	Commercial service that provides chemical information for US and Global regulations. Contains chemical, physical and toxicity information	NA	
Infochem database	<a href="http://www.infochems.com/main/default.asp">http://www.infochems.com/main/default.asp</a>	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	 <p><b>MTC Libraries</b> Managerial Technologies Corp Resource Libraries</p> <p>The Business Library The HR Library rmLibrary The Safety Library The Healthcare Library The Transportation Library</p>	Libraries Overview	Subscribe
What They Say About Us	What's New		Referral Programs	About Us
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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# ECOTOX Database

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[EPA Home](#) > [ECOTOX](#) > Basic Search

## Quick Database Query ?

### 1 Select Query Parameters

Scroll to or click on [Chemical](#),  
[Taxonomic](#), [Effect](#), [Publication Years](#)

### 2 Select Report Format

Scroll to or click on [Report Format](#)

### 3 Perform Query

Click on Perform Query for Aquatic Data  
or Perform Query for Terrestrial Data  
buttons under Key Functions box

#### KEY FUNCTIONS

[Restore Defaults](#)

[Perform Query  
for Aquatic Data](#)

[Perform Query  
for Terrestrial Data](#)

#### Chemical Entry ?

[Clear Selections](#)

**Search Tip:** [Browse Chemical Index](#) to find the best input format for your chemical information.

Enter either chemical names and/or CAS Registry numbers below. The system allows for both chemical names and CAS numbers to be entered in the same query. Place each individual entry on a separate line. To ensure your final entry is included, end your selection list with a final return (enter key).

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- Name=Struct

Enter a Chemical Name, CAS Number, Molecular Formula or Weight.  
Use \* for partial names (e.g. ben\*).  
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Please contact [databases@cambridgesoft.com](mailto:databases@cambridgesoft.com) for enterprise subscription information.

### Reference Databases

ChemFinder	FREE	<a href="#">Search</a>	<a href="#">About</a>
ChemINDEX		<a href="#">Search</a>	<a href="#">About</a> <a href="#">Trial</a>
Name=Struct		<a href="#">Search</a>	<a href="#">About</a>
NCI		<a href="#">Search</a>	<a href="#">About</a> <a href="#">Trial</a>
The Merck Index		<a href="#">Search</a>	<a href="#">About</a> <a href="#">Trial</a>
Ashgate Drugs		<a href="#">Search</a>	<a href="#">About</a> <a href="#">Trial</a>

### Chemical Databases

ChemACX Pro	<a href="#">Search</a>	<a href="#">About</a>	<a href="#">Trial</a>
ChemACX Pro & ChemACX-SC Pro	CD only	<a href="#">About</a>	

### Reaction Databases

Organic Syntheses	FREE	<a href="#">Search</a>	<a href="#">About</a>
ChemReact500		<a href="#">Search</a>	<a href="#">About</a> <a href="#">Trial</a>
ChemReact68		<a href="#">Search</a>	<a href="#">About</a> <a href="#">Trial</a>



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**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.

[Section 8\(e\) 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.  
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[dmiletech.com](http://dmiletech.com)

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**Click here to learn how**

# Modeling & Assessment Programs

Modeling Programs- Assessment Tools					
Data Base	URL	Source	Comment		
PBT Profiler	<a href="http://www.pbtprofiler.net/">http://www.pbtprofiler.net/</a>	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)	<a href="http://www.epa.gov/oppt/newchems/tools/21ecosar.htm">http://www.epa.gov/oppt/newchems/tools/21ecosar.htm</a>	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	<a href="http://www.epa.gov/opptintr/exposure/pubs/gems.htm">http://www.epa.gov/opptintr/exposure/pubs/gems.htm</a>	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	<a href="http://www.epa.gov/opptintr/exposure/pubs/episuite.htm">http://www.epa.gov/opptintr/exposure/pubs/episuite.htm</a>	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	<a href="http://www.epa.gov/opptintr/exposure/docs/efast.htm">http://www.epa.gov/opptintr/exposure/docs/efast.htm</a>	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	

# EPA's PBT Profiler



[Methodology](#) · [Criteria](#) · [Definitions](#) · [Chemicals That Should Not be Profiled](#)  
[Home](#) · [Start a New Profile](#) · [Results](#) · [Terms of Use](#) · [Security](#)

## Results

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

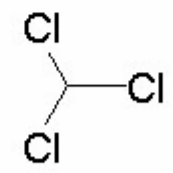
[Persistence](#)

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

**67-66-3 Methane, trichloro-**

**PBT Profiler Estimate = PBT**

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



[P2 Considerations and more information](#)

Start a New Profile

Add More Chemicals to Your Profile

The PBT Profiler Results are available for 20 minutes



The image is a screenshot of a web browser displaying the EPA's New Chemicals Program website. The browser's address bar shows the URL: http://www.epa.gov/oppt/newchems/tools/21ecosar.htm. The page header features the U.S. Environmental Protection Agency logo and the title "New Chemicals Program". A search bar with a "GO" button is present. A breadcrumb trail reads: EPA Home &gt; Prevention, Pesticides &amp; Toxic Substances &gt; Pollution, Prevention &amp; Toxics &gt; New Chemicals Program &gt; ECOSAR. The main heading is "Ecological Structure Activity Relationships". Below this, there is a small image of a computer monitor and keyboard, with the text "v. 0.99g, January, 2000" next to it. The page contains three sections: "What is ECOSAR?", "What is a Structure Activity Relationship (SAR)?", and "How Does ECOSAR Work?". The left sidebar contains a navigation menu with links to "Chemicals homepage", "Forms and Information", "Manufacture Notice Status", "Chemicals Policies", "Hazardous Materials", "Chemical Categories Report", "Significant New Use Rules", "ECOSAR: Ecological Structure Activity Relationships", and "Reporting and Submitting New Chemicals". The bottom of the browser window shows the "Internet" icon.

## New Chemicals Program

[Contact Us](#) | [Print Version](#) Search:  [GO](#)

[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?

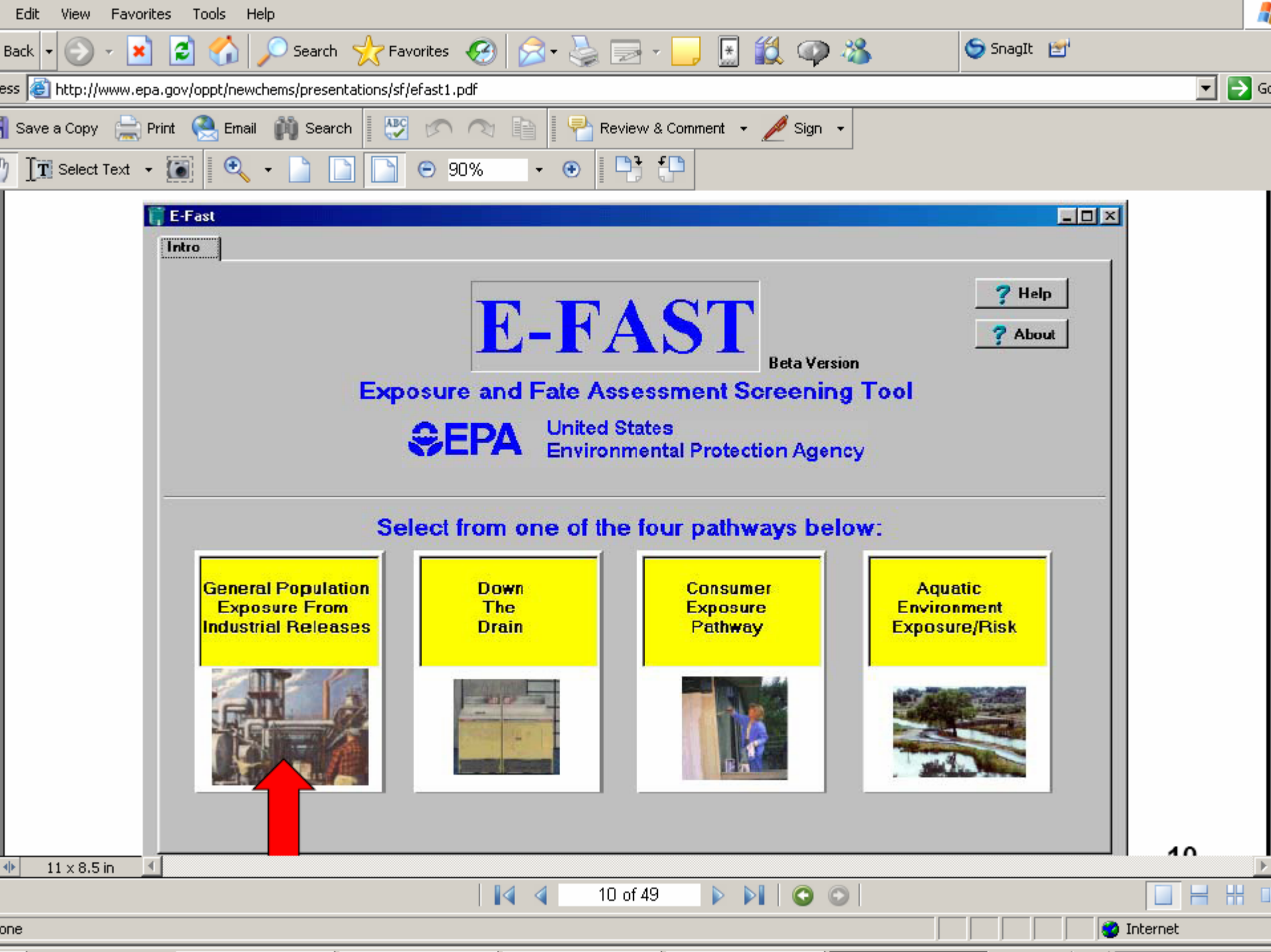
ECOSAR (Ecological Structure Activity Relationships) is a personal computer software program that is used to estimate the toxicity of chemicals used in industry and discharged into water. The program predicts the toxicity of industrial chemicals to aquatic organisms such as fish, invertebrates, and algae 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.



E-Fast

Intro

# E-FAST

Beta Version

## Exposure and Fate Assessment Screening Tool



? Help  
? About

Select from one of the four pathways below:

**General Population Exposure From Industrial Releases**

**Down The Drain**

**Consumer Exposure Pathway**

**Aquatic Environment Exposure/Risk**



# 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 more powerful tool 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.