

# **ECOTOX Knowledgebase**

Chris Russom





### What is ECOTOX?

- ECOTOX is a comprehensive database summarizing the toxicity of single chemicals to aquatic and terrestrial organisms
- Available on Internet (www.epa.gov/ecotox)
- Developed and maintained by ORD/NHEERL/MED
- ECOTOX includes test results published in the open literature, and from other government data sources
- All pertinent information on the species, chemical, test methods, and results are abstracted and encoded into the database
- ECOTOX is internationally recognized as the source for ecotoxicological data



#### Is ECOTOX an "Eco-IRIS"

- Yes and No
- Both ECOTOX and IRIS are considered to be comprehensive and authoritative sources
- However:
  - ECOTOX provides, but does not interpret data
  - ECOTOX can access data in many ways; e.g., by chemical, species, endpoint, route of exposure etc.



# **ECOTOX Supports Efficiency and Transparency in Regulatory Decision-Making**

- Supports EPA's:
  - Risk Characterizations: Transparency, Clarity, Consistency
  - Information quality guideline provisions
  - Responsible use of Agency resources



### Requirements for Inclusion in ECOTOX

- Single chemical exposure with verifiable CAS Registry number
- Taxonomic information for species can be verified
- Studies on live organisms
- Observed effect with concurrent exposure information (dose / concentration / application rate)
- Study / exposure duration is reported
- Sediment exposures are included if water concentration is provided
- Full-text articles published in a language other than English
- Publication is the primary source of the data

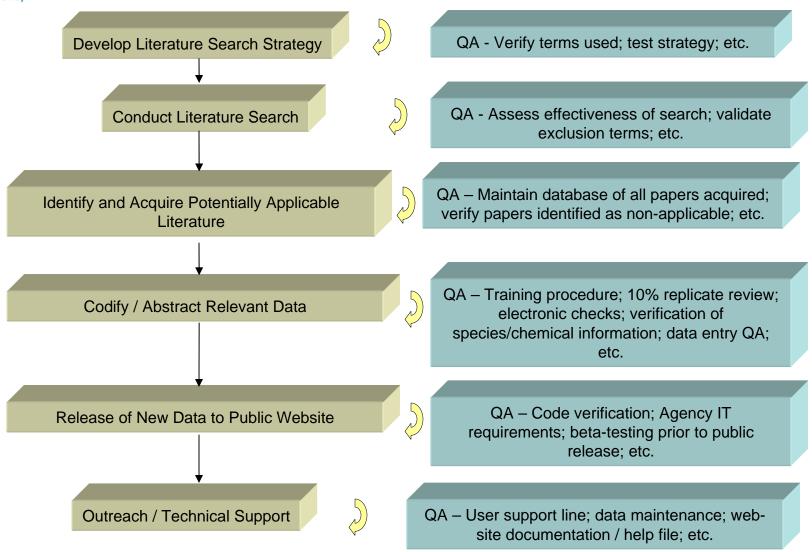


#### What studies are excluded?

- Mixture studies (formulated products are included)
- Petroleum/fuel products
- Air pollution studies
- Inhalation studies for terrestrial animals
- Studies using dead organisms
- in vitro studies
- Studies that do not report a duration of exposure
- Abstracts
- Full-text non-English publications
- Review articles



### **Procedures used in development of ECOTOX**





# Figure 1: Data fields coded within ECOTOX from studies

#### Chemical **Methods** Results Source of Data **Species** Full Citation Application CAS Registry No. Common Name Route of Exposure Major Effect Frequency / Presented for Category (e.g., Collective Date / Rate Each Test Scientific Name **Exposure Media** Enzvme Indices Name Result Habitat Study / Taxonomic Observed Description for Contact Synonyms Hierarchy Exposure Effect Field Studies Information for Duration Measurements Data Steward Chemical Form Organism Age Longitude / (e.g., P450 for each Third-**Application** Latitude for Enzyme Party Data File **Chemical Purity** Organism Sex Frequency Response Field Studies Solvent / **Initial Weight** Study Location Calculated and Length Vehicle Used **Endpoints** Water / Soil (e.g., EC50) Initial Life Chemical Class Chemistry Stage Dose Other Control Type Response Comments on (Terrestrial Organism Studies only) Chemical Noted by Concentration Information % Effect Author Response Comments on Experimental Design Statistical Info



### ECOTOX - data released / coded in last year

- Database updated in March 2008 and December 2008 (increase in past year in parenthesis)
  - Currently system covers
    - 8894 chemical (+128)
    - 7997 species (+824)
    - 27,759 publications (+3507)
    - 7 electronic data files (EPA, USGS, OECD, Russia)
    - 614,090 individual test results (+54,912)
  - Focus this year was on comprehensively coding all published data, meeting acceptance criteria for 95 specific chemicals and their degradates
  - Next data release scheduled for mid-February



# **Program Offices & Regions Applications**

- Site specific ecological risk assessments
- Development of benchmarks



 Ecological Soil Screening Levels, Water Quality Criteria, Toxicity Reference Values, Water Quality Standards

- RCRA facility permits
- Emergency Response
- Pesticide registrations/re-registrations
- **Endangered Species Act counterpart regulation**
- Ranking / prioritization exercises
- Industrial chemical reviews
- Toxicity weighting factors for effluent guidelines
- NPDES permits and TMDLs









## How do we prioritize data abstraction and review?

- We focus on studies:
  - That include data for chemicals prioritized by ORD and Program Offices
  - Having acceptable controls
  - Where test results are statistically analyzed



## ECOTOX – data released / coded in last year

	T	<u> </u>	
Abscisic Acid	Disulfoton	Methidathion	Quizalofop-ethyl
Acephate	Diuron	Methoprene	Rotenone
Acetic acid	EDTA, Iron (III) salt	Naled	Silica dioxide / silica
Aldicarb	EPTC	Natamycin	Soap salts
Azadirachtin	Ethoprop	Neem oil (Azadirachta indica)	Sodium Fluoride
Azinphos-methyl	Ethylenethiourea	Nerolidol	Sodium perborate
Bensulide	Ethynyl estradiol	Nicotine	Sodium propionate
Biobor	Farnesol	Nithiazine	Sodium Tetrathiocarbonate
Busan 1024	Fenamiphos	Nonylphenol	Streptomycin
Calcium propionate	Flumetsulam	Norflurazon	Sulfur
Calcium tetrathiocarbonate	Flutolanil	Oregano oil	Temephos
Carbon dioxide	Fosetyl-Al	Oxamyl	Terbufos
Carbon disulfide	Glufosinate	Oxazolidine-E	Tetrachlorvinphos
Chitin	Glyphosate	Oxydemeton-methyl	Thiencarbazone-methyl
Chlorthal-dimethyl	Homobrassinolide	Oxyfluorfen	Trenbolone
Citric acid	Imidacloprid	Oxytetracycline	Tribufos
Clethodim	Indole	Permethrins	Tributyl Tin
Coumaphos	Inorganic nitrate	Phorate	Trimethoxysilyl quats
Cumyluron	Iodide	Pirimiphos-methyl	Trinexapac-ethyl
Cyanamide	Iron salts	Profenofos	Zinc Borate
Cyprosulfamide	Isoxaben	Propargite	Zinc salts
Diazinon	L-Lactic acid	Propetamphos	Ziram
Dicrotophos	Mancozeb	Propionic Acid	
Dimethoate	Methamidophos	Quinclorac	
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### ECOTOX – chemicals scheduled in 2009

1RS, cis-Permethrin 2-Mercaptobenzothiazole Aldicarb Aliphatic alcohols, C1-C5 Allethrin stereoisomers Amitraz Ammonia Atonik Azoxystrobin Bentazon Bifenthrin Boll weevil attractants Bromohydroxyacetophenone Capsaicin Carbaryl Carbofuran Chlorfenapyr Chlorpyrifos	Decyl isononyl dimethyl ammonium chloride Deltamethrin Dibromo-3-nitrilopropionamide Dichromic acid Difenzoquat Diflubenzuron Diquat Dibromide Disodium cyanodithioimidoca Dowicil 100 Esfenvalerate Ethephon Ethylene Fenpropathrin Fluazinam Flumiclorac Fluridone Flurprimidol	Hexaflumuron Hexazinone IBA Inorganic halides Iprodione Limonene Linuron Maleic Hydrazide meta-Cresol Metalaxyl Methiocarb Methomyl Mineral acids Nanomaterials Napthenate salts OBPA (10, 10'- Oxybisphenoxarsine) Oxamyl	Pirimicarb Polybutene resins Pronamide Propoxur Pyridaben Sodium cyanide Strychnine Sulfentrazone Tebuthiuron Terbuthylazine Thiobencarb Thiodicarb Thymol Tralomethrin Triclopyr Trifluralin Tris(HOCH2-)nitromethane Vegetable and flower oils
Bromohydroxyacetophenone Capsaicin Carbaryl Carbofuran Chlorfenapyr	Ethylene Fenpropathrin Fluazinam Flumiclorac Fluridone	Mineral acids Nanomaterials Napthenate salts OBPA (10, 10'- Oxybisphenoxarsine)	Thymol Tralomethrin Triclopyr Trifluralin Tris(HOCH2-)nitromethane





#### **Ecological Soil Screening Levels**

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Eco-SSL Guidance Documents and SOPs

Literature Identification

Tools

Interim Eco-SSLs FAQ

The EPA Web site is undergoing technical testing this weekend. Some services will be unavailable intermittently between 8:00 am and 5:00 pm ET Saturday, January 24. We apologize for any inconvenience.

#### **ECO-SSL**

The Ecological Soil Screening Level (Eco-SSL) derivation process represents the collaborative effort of a multi-stakeholder workgroup consisting of federal, state, consulting, industry and academic participants led by the U.S. EPA, Office of Emergency and Remedial Response. It is emphasized that the Eco-SSLs are soil screening numbers, and as such are not appropriate for use as cleanup levels. Screening ecotoxicity values are derived to avoid underestimating risk. Requiring a cleanup based solely on Eco-SSL values would not be technically defensible.

The Eco-SSL web site provides an overview of the contaminant. Separate discussion are provided for each receptor group including a comprehensive list of literature evaluated under the effort, and a summary of data used in deriving Eco-SSL values. For each chemical, Eco-SSL documents are provided in a PDF format which requires the Acrobat Reader. For some documents HTML versions are available with linkages to the toxicity data records within the U.S. EPA's ECOTOX database.

#### Interim Eco-SSL Documents

#### METALS

Aluminum PDF (297KB) Antimony PDF (981KB) Arsenic PDF (1,725KB) Barium PDF (1,238KB) Beryllium PDF (1,098KB) Cadmium PDF (2,591KB)

Chromium PDF (563KB) UPDATED 5/08 Cobalt PDF (1,775KB)

Copper PDF (1,743KB) UPDATED 2/07

Iron PDF (439KB) Lead PDF (1,466KB)

Manganese PDF (1,466KB) NEW 7/07

Nickel PDF (830KB) NEW 3/07 Selenium PDF (1,061KB) NEW 11/07 Silver PDF (652KB) NEW 9/06

Vanadium PDF (1,939KB) Zinc PDF (4,857KB) NEW 11/07

#### ORGANICS

DDT and metabolites PDF (922KB) NEW 8/07 Dieldrin PDF (787KB) UPDATED 10/07 Pentachlorophenol PDF (699KB) UPDATED 8/07 Total PAHs PDF (1,758KB) NEW 8/07

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Last updated on Wednesday, May 21st, 2008. http://www.epa.gov/ecotox/ecossl/

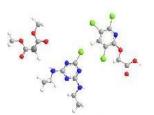




#### ASTER - Assessment Tools for the Evaluation of Risk

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ASTER Single Chemical Processing



U.S. ENVIRONMENTAL PROTECTION AGENCY

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Tools

3rd Party Software

Limitations

Frequently Asked Questions

**ECOTOX** 

**Browse Chemicals** 

ASTER (Assessment Tools for the Evaluation of Risk) was developed by the U.S. EPA Mid-Continent Ecology Division, Duluth, MN (MED-Duluth) to assist regulators in performing ecological risk assessments, ASTER is an integration of the ECOTOXicology Database (ECOTOX) and the QSAR (Quantitative Structure Activity Relationships) system, a structure activity based expert system. ASTER is designed to provide high quality data for discrete chemicals, when available in the associated databases and QSAR-based estimates when data are lacking. The QSAR system includes a database of measured physicochemical properties such as melting point, boiling point, vapor pressure, and water solubility as well as more than 56,000 molecular structures stored as SMILES (Simplified Molecular Input Line Entry System) strings for specific chemicals, ECOTOX is a comprehensive database, which provides information on adverse effects of single chemical stressors to ecologically relevant aquatic and terrestrial species. ECOTOX includes more than 500,000 test records covering more than 6,000 aguatic and terrestrial species and 10,000 chemicals.

Prior to using ASTER, we suggest you visit the ASTER HELP section of this web site, for guidance on ASTER and writing SMILES strings.

Supporting modules were also provided by U.S.EPA Office of Pollution Prevention and Toxics (KowWin & BioWin), Bourgas Prof. Assen, Zlatarov University EXIT Disclaimer (2-D structure depiction software), and BioByte Corporation EXIT Disclaimer (ClogP).

You should consult the original scientific paper to ensure an understanding of the context of the data retrieved from the ECOTOX database.

The chemical property calculation for pKa is not fully functional. Currently, the pKa is only being calculated for phenol compounds. Additional pKa calculations will be implemented in future versions of ASTER.

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