

Computational research methods/models/ tools/databases for health and ecological risk assessments – continued

Jennifer Olker
olker.jennifer@epa.gov

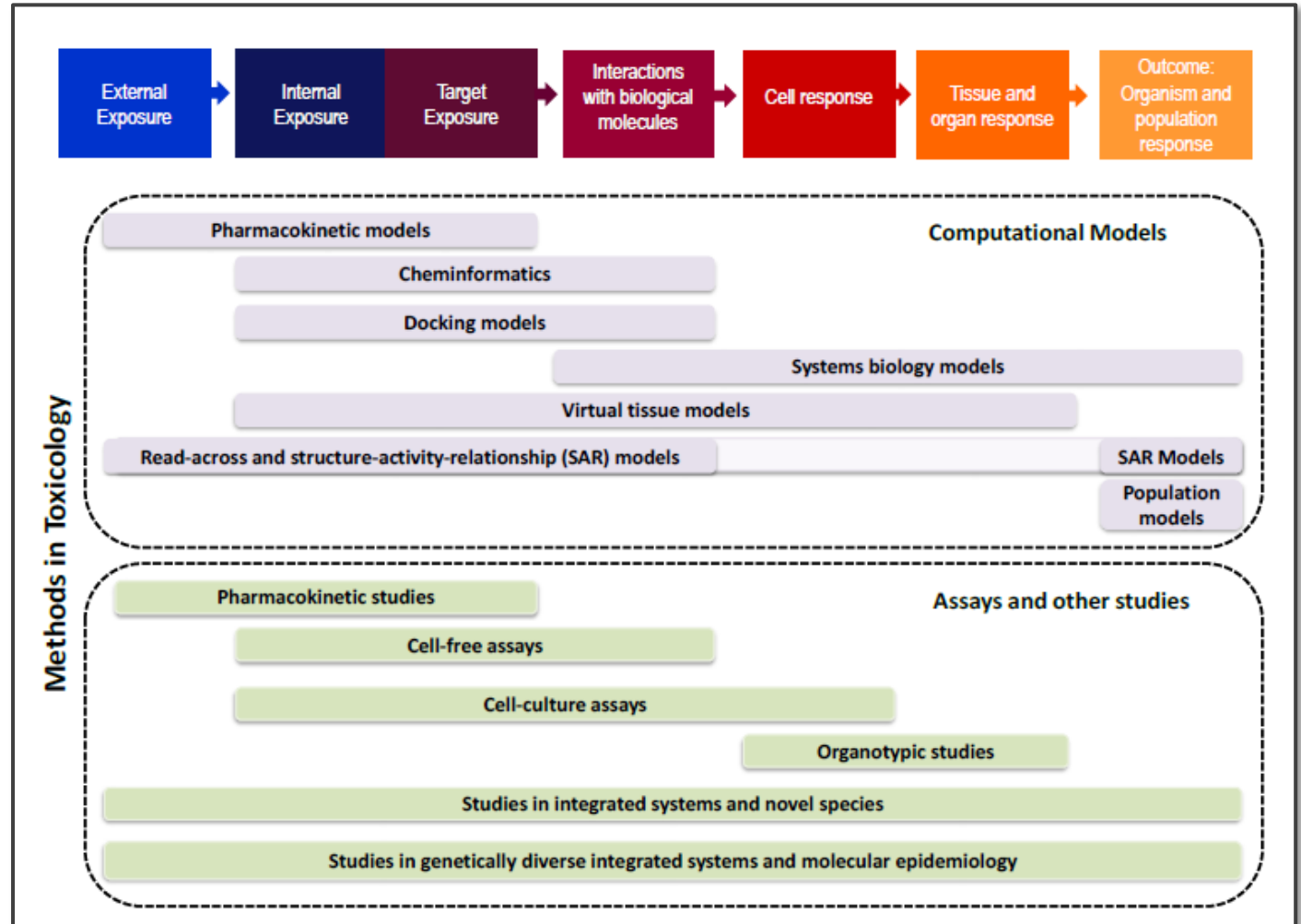
*Center for Computational Toxicology & Exposure
US EPA Office of Research and Development (ORD)*

**Georgetown University
EMAP Program
April 2021**

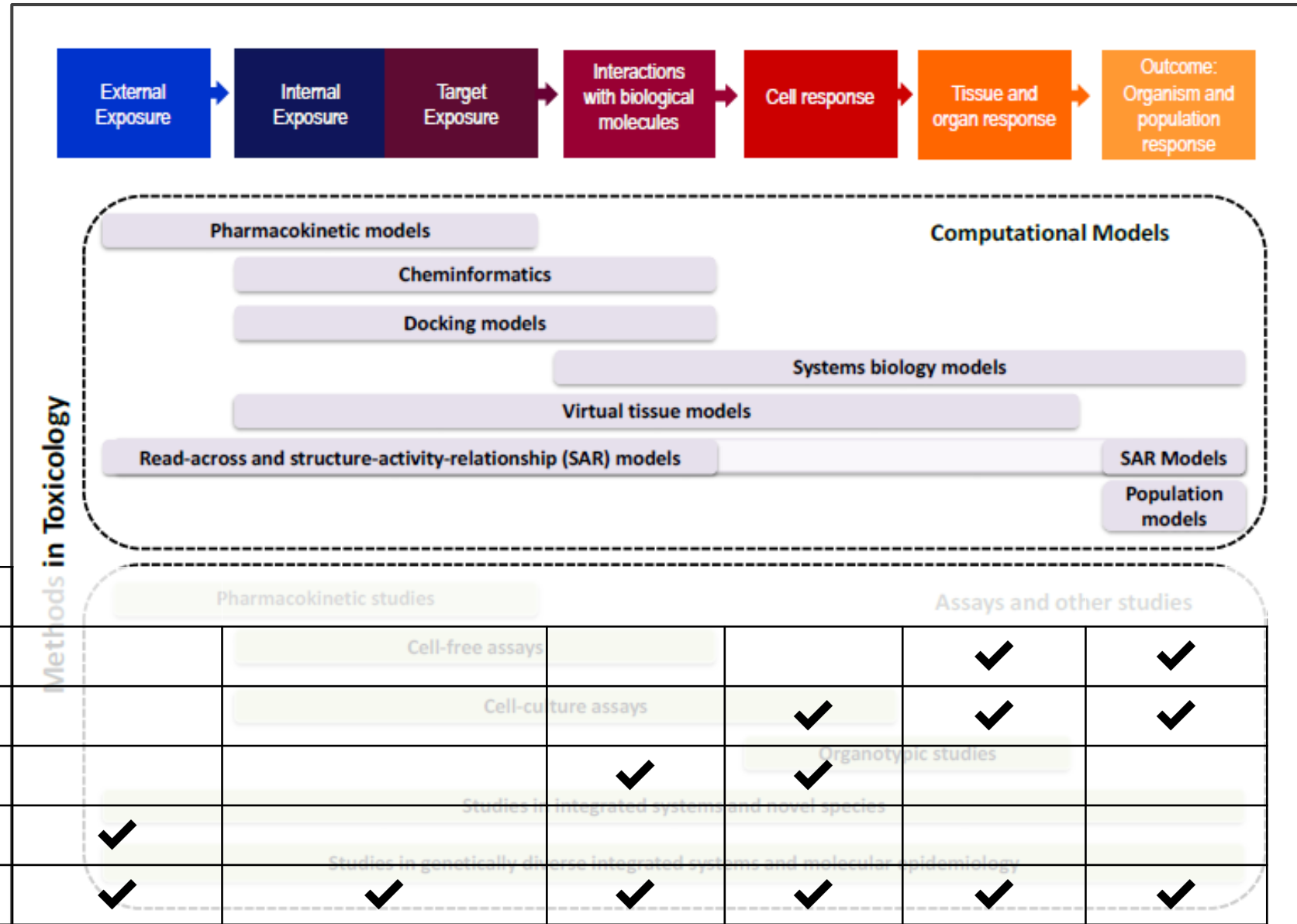
Toxicology Moving to Embrace 21st Century Methods



<https://www.nap.edu/catalog/24635/using-21st-century-science-to-improve-risk-related-evaluations>



Data Sources and Tools



Data Sources and Tools

Source	External Exposure	Internal Exposure	Target Exposure	Interactions with biological molecules	Cell response	Tissue and organ response	Outcome: Organism and population response
CompTox Chemicals Dashboard	✓	✓	✓	✓	✓	✓	✓
httk	✓	✓	✓				
OPERA	✓						
SSD Toolbox							✓
EcoSAR							✓
McNest							✓
Toxicity Translators							✓
ToxRefDB						✓	✓
ECOTOX KB					✓	✓	✓
InVitro DB				✓	✓		
CPDat	✓						
Open Literature	✓	✓		✓	✓	✓	✓

Data Sources and Tools

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CompTox Chemicals Dashboard	✓	✓	✓	✓	✓	✓	✓	Multiple Species
httk	✓	✓	✓					
OPERA	✓							
SSD Toolbox							✓	
EcoSAR							✓	Populations
McNest							✓	
Toxicity Translators							✓	
ToxRefDB						✓	✓	Multiple Species
ECOTOX KB					✓	✓	✓	
InVitro DB				✓	✓			
CPDat	✓							
Open Literature	✓	✓	✓	✓	✓	✓	✓	

CompTox Chemicals Dashboard

<https://comptox.epa.gov/dashboard>



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CompTox Chemicals Dashboard

883 Thousand Chemicals

[Window Snip](#)

Chemicals

Product/Use Categories

Assay/Gene



Search for chemical by systematic name, synonym, CAS number, DTXSID or InChIKey

☐ Identifier substring search

See what people are saying, read the dashboard [comments!](#)

Cite the Dashboard Publication [click here](#)

Latest News

[Read more news](#)

New article to help understand the Batch Search functionality published

March 22nd, 2021 at 3:21:30 PM

A new article regarding the [batch search](#) on the Dashboard is described in a recent article in the Journal of Chemical Information and Modeling:
[Enabling High-Throughput Searches for Multiple Chemical Data Using the U.S.-EPA CompTox Chemicals Dashboard.](#)


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883 Thousand Chemicals

Chemicals	Product/Use Categories	Assay/Gene
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☐ Identifier substring search

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New article to help u

March 22nd, 2021 at 3:21:30 PM

A new article regarding the [batch](#)
[Enabling High-Throughput Search](#)

DETAILS

EXECUTIVE SUMMARY

PROPERTIES

ENV. FATE/TRANSPORT

HAZARD

► SAFETY

► ADME

▶ EXPOSURE

▶ BIOACTIVITY

SIMILAR COMPOUNDS

GENRA (BETA)

RELATED SUBSTANCES

SYNONYMS

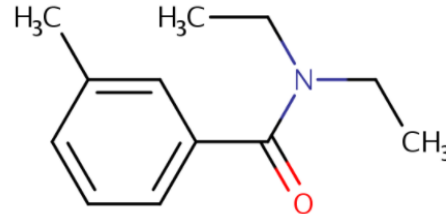
► LITERATURE

LINKS



134-62-3 | DTXSID2021995

Searched by DSSTox Substance Id.



Wikipedia

***N,N*-Diethyl-*meta*-toluamide**, also called **DEET** () or **diethyltoluamide**, is the most common active ingredient in insect repellents. It is a slightly yellow oil intended to be applied to the skin or to clothing and provides protection against mosquitoes, ticks, fleas, chiggers, leeches and many biting insects.

[Read more](#)

Quality Control Notes

Intrinsic Properties

 Molecular Formula: C₁₂H₁₇NO
 Mol File
 Find All Chemicals

 Average Mass: 191.274 g/mol **Isotope Mass Distribution**

 Monoisotopic Mass: 191.131014 g/mol

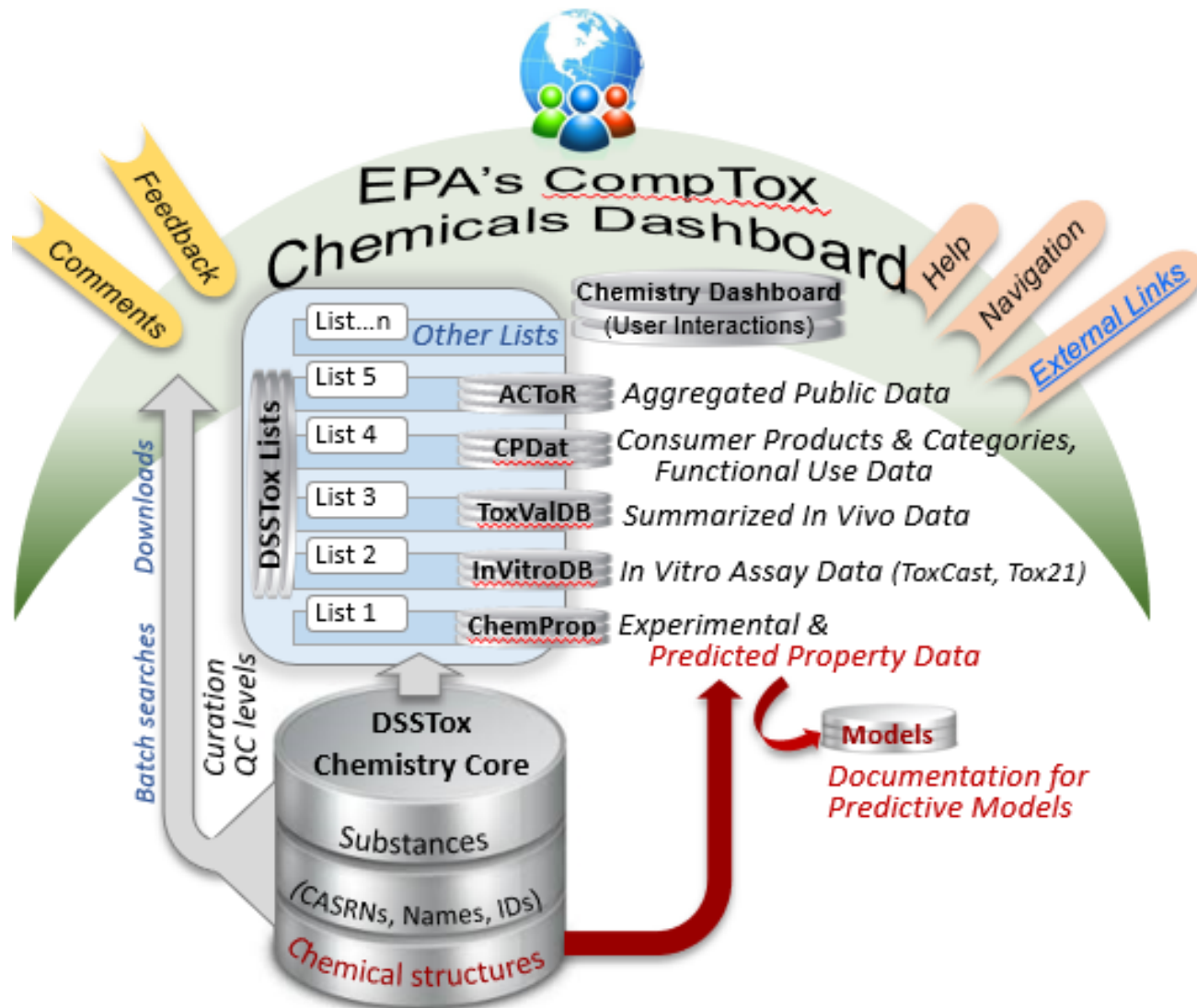
Structural Identifiers

Linked Substances

Presence in Lists

Record Information


CompTox Chemicals Dashboard



- Integration of multiple databases
 - DSSTox substance database
 - ToxValDB (includes ToxRef & ECOTOX)
 - CPCat and CPDat consumer products
 - InvitroDB (ToxCast/Tox21)
 - Property Database
 - QSAR predicted data
- Integrated to other Sources
 - Toxics Release Inventory
 - IRIS Reports
 - PPRTV Reports
 - ChemView
 - EPA Substance Registry Service
 - AOP-Wiki
- Links to ~80 public sites & services

CompTox Chemicals Dashboard

<https://comptox.epa.gov/dashboard>



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883 Thousand Chemicals

SEARCH

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[Product/Use Categories](#)
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☐ Identifier substring search



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DEET

134-62-3 | DTXSID2021995

Searched by DSSTox Substance Id.



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- PROPERTIES
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- HAZARD
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...

[Read more](#)

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  Mol File
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  Isotope Mass Distribution

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March 22nd, 2021 at 3:21:30 PM


A new article regarding the [batch Enabling High-Throughput Sear](#)

CompTox Chemicals Dashboard

<https://comptox.epa.gov/dashboard>


**DEET**
134-62-3 | DTXSID2021
Searched by DSSTox Substance Id

- DETAILS
- EXECUTIVE SUMMARY
- PROPERTIES
- ENV. FATE/TRANSPORT
- HAZARD
- SAFETY
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**DEET**
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Searched by DSSTox Substance Id


Summary

Property	Experimental average	Predicted average	Experimental median	Predicted median	Experimental range	Predicted range	Unit
LogKow: Octanol-Water	2.18 (1)	2.16		2.21	2.18	1.96 to 2.26	-
Melting Point	-45.0 (3)	26.6	-45.0	38.4	-45.0	-44.4 to 85.7	°C

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Searched by DSSTox Substance Id

Hazard


Human Eco

**DEET**
134-62-3 | DTXSID2021995
Searched by Approved Name.

Chemical Activity Summary

BIOACTIVITY

Species	Subsource	Source
rat	Japan NITE	HESS
rat	Japan NITE	HESS
rat	Japan NITE	HESS
rat	Japan NITE	HESS
rat	Japan NITE	HESS
rat	EPA ORD	ToxRefDB
rat	EPA ORD	ToxRefDB
rat	EPA ORD	ToxRefDB

**DEET**
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Searched by Approved Name.

Product and Use Categories (PUCs)

Product or Use Categorization	Categorization type	Number of Unique Products
insect repellent: insect repellent - skin	PUC	49
Not Yet Categorized:	PUC	37
insect repellent:	PUC	7
	PUC	6
detected, drinking water	CPCat Cassette	2
insecticide:	PUC	2
active ingredient, Australia	CPCat Cassette	1
active ingredient, Pesticides	CPCat Cassette	1
Canada, consumer product, Substances in Products - Canada	CPCat Cassette	1
pharmaceutical	CPCat Cassette	1


10 records

ASSAY DETAILS

ACSO (uM) 0.18
Scaled top: 1.08
Assay Endpoint Name: LFEA_HepaRG_GADD45G_up
Gene Symbol: GADD45G
Organism: human
Tissue: liver
Assay Format Type: cell-based
Biological Process Target: regulation of transcription factor activity
Detection Technology: Fluidigm qRT-PCR
Analysis Direction: positive
Intended Target Family: mutagenicity response
Description: Change in transcription factor expression relative to control (delta-delta-ct) for HepaRG cell cultures in an induction preparation. The adherent cells have some metabolic capability. Expression measured by inducible reporter assay using Fluidigm qRT-PCR to monitor. Suffix _up indicates curve fitting for increase in expression (induction).

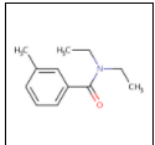
CompTox Chemicals Dashboard

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DETAILS

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LITERATURE

LINKS

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607 chemicals

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SAFETY

ADME

EXPOSURE

BIOACTIVITY

SIMILARITY

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Abstract Sifter

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Authors	Journal	Rev
U. Harada	Regulatory toxicology and pharmacology : RTP	
Batter, O'Dell, Syed, Wheeler, Debb.	Journal of medical entomology	
Nadeem, Ali, Ahmad, Anwar, Mustaf.	Journal of Ayub Medical College, Abbottabad : JAMC	
vic	Journal of hazardous materials	
Fildier, Libert, Groud, Hammada, H.	The Science of the total environment	
ada, Kuramoto, Mitsuhashi, Saitoh, ...	Parasites & vectors	
Shao, He, Zhang, Jia	Journal of environmental science and health. Part. ...	
Jankowski, Ferrey, Chenaux-Ibrahi.	The Science of the total environment	
enas, Affy, Yilmaz, Potter, Laminett.	Current biology : CB	
ente, Cuba, Allen, Becnel, Linticum	Journal of the American Mosquito Control Association	
ffe, MacKenzie	Journal of the American Mosquito Control Association	
g, Focke, Boldt, Androsch, Leuteritz	The Journal of dermatology	
	Materials (Basel, Switzerland)	

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LINKS

General

EPA Substance Registry Service

PubChem

ChemSpider

CPCat

DrugBank

Wikipedia

MSDS Lookup

CHEMBL

ToxPlanet

ACS Reagent Chemicals

Wolfram Alpha

ECHA Infocard

ChemAgora

Consumer Product Information Database

CHEBI

NIST Chemistry Webbook

WEBWISER

PubChem Safety Sheet

Consumer Product Information Database

PubChem: Chemical Vendors

CAMEO Chemicals

Toxicology

ACToR

DrugPortal

CCRIS

ChemView

CTD

eChemPortal

Gene-Tox

HSDB

ACToR PDF Report

CREST

National Air Toxics Assessment

ChemView

Chemical Checker

BindingDB

CaEPA OEHHHA

NIOSH IDLH Values

LactMed

ECOTOX

Publications

Toxline

PPRTVWEB

PubMed

IRIS Assessments

EPA HERO

NIOSH Skin Notation Profiles

NIOSH Pocket Guide

RSC Publications

BioCaddie DataMed

Springer Materials

Bielefeld Academic Search Engine

CORE Literature Search

Google Books (Text Search)

Google Patents (Text search)

Google Scholar (Text search)

Google Patents (Structure search)

Google Books (Structure Search)

Google Scholar (Structure search)

Federal Register

Analytical

RSC Analytical Abstracts

Tox21 Analytical Data

MONA: MassBank North America

mzCloud

NIST IR Spectrum

NIST MS Spectrum

MassBank

NIST Antoine Constants

IR Spectra on PubChem

NIST Kovats Index values

Protein DataBank

National Environmental Methods Index

Prediction

2D NMR HSQC/HMBC Prediction

Carbon-13 NMR Prediction


Proton NMR Prediction

ChemRTP Predictor

LSERD

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Search queryCopy page URL

List Acronym ▼	List Name ▼	Last Updated ▼	Number of Chemicals ▼	List Description ▼
40CFR1164	40CFR116.4 Designation of Hazardous Substances (Above Ground Storage Tanks)	2020-06-25	331	Hazardous Substance List (40CFR116.4): related to Above Ground Storage Tanks
40CFR355	40CFR355 Extremely Hazardous Substance List and Threshold Planning Quantities	2018-01-05	354	Extremely Hazardous Substance List and Threshold Planning Quantities; Emergency Planning and Release Notification Requirements; Final Rule. (52 FR 13378)
ACSREAG	LIST: ACS Reagent Chemicals	2017-04-14	405	The ACS Committee on Analytical Reagents sets purity specifications for almost 500 reagent chemicals and over 500 standard-grade reference materials.
AEGLVALUES	AEGLS: Acute Exposure Guideline Levels	2018-04-20	174	Acute exposure guideline levels (AEGLs) describe the human health effects from once-in-a-lifetime, or rare, exposure to airborne chemicals.
ALGALTOX	LIST: Algal Toxins	2018-05-04	55	A list of Algal Toxins of potential interest
ALLSURFACTANTS	CATEGORY: Surfactants	2020-10-28	805	A set of surfactants made from the assembly of multiple surfactants list
AMINOACIDS	CATEGORY: Amino acids	2019-02-04	20	Amino acids are organic compounds containing amine (-NH2) and carboxyl (-COOH) functional groups, along with a side chain (R group) specific to each amino acid.
AMPHIBOLES	LIST: Amphiboles	2019-03-26	23	Amphiboles are an important group of inosilicate minerals.
ANTIBIOTICS	CATEGORY PHARMACEUTICALS: Antibiotics	2019-11-16	170	List of antibiotics and related compounds
ANTIMICROBIALS	CATEGORY WIKILIST ANTIMICROBIALS: List of Antimicrobials from Wikipedia	2020-10-11	289	A list of antimicrobials extracted from Wikipedia.

First<<<12345678910>>>Last

Showing 1 to 10 of 297 records

LITERATURELINKS

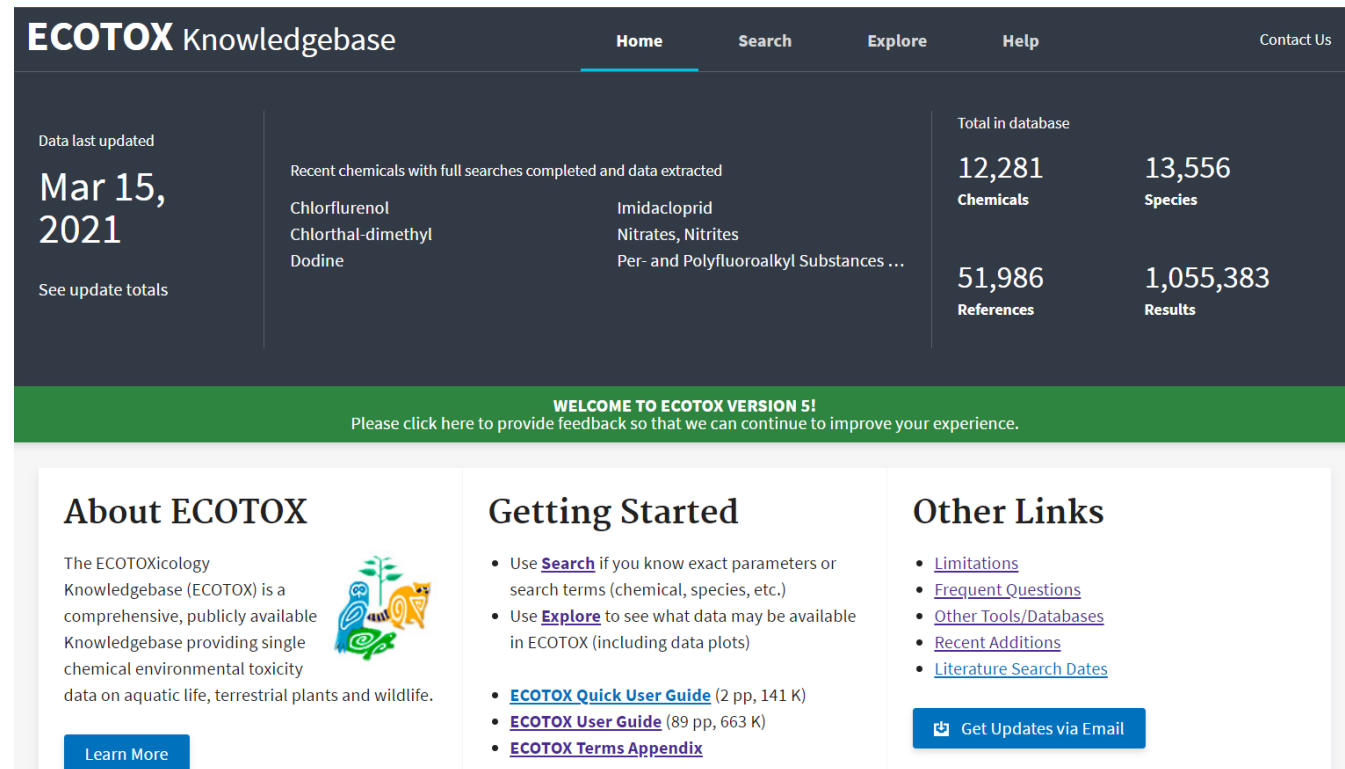
Other

LIST: BLOODEXPOSOMECATEGORY|COSMETICS: COSMOS DB cosmetics databaseEPA|LIST: Article "Workflow for Defining Reference Chemicals for Assessing Performance of In Vitro Assays"LIST: Chemicals in biosolidsNORMAN: REACH Chemicals List Provided to NORMAN NetworkMASSSPEC: CASMI2016 Training datasetNORMAN: Norman Network Suspect Screening List (SUSDAT)

ECOTOX Knowledgebase

Publicly available, curated database providing toxicity data from single-chemical exposure studies to aquatic life, terrestrial plants and wildlife

- From comprehensive search and review of open and grey literature
 - Data extracted from acceptable studies, with up to 250 fields
 - Updated quarterly to public website
- 30+ year history
 - Originated in the early 1980s
 - Developed at US EPA's Office of Research and Development in Duluth
- Current user statistics
 - 8,000 distinct hosts search the Knowledgebase each month




ECOTOX Knowledgebase Home Search Explore Help Contact Us

Data last updated Mar 15, 2021 See update totals	Recent chemicals with full searches completed and data extracted Chlorlurenol Chlorthal-dimethyl Diodine Imidacloprid Nitrates, Nitrites Per- and Polyfluoroalkyl Substances ...	Total in database 12,281 Chemicals 13,556 Species 51,986 References 1,055,383 Results
---	--	---

WELCOME TO ECOTOX VERSION 5!
Please click here to provide feedback so that we can continue to improve your experience.

About ECOTOX

The ECOTOXicology Knowledgebase (ECOTOX) is a comprehensive, publicly available Knowledgebase providing single chemical environmental toxicity data on aquatic life, terrestrial plants and wildlife.



[Learn More](#)

Getting Started

- Use [Search](#) if you know exact parameters or search terms (chemical, species, etc.)
- Use [Explore](#) to see what data may be available in ECOTOX (including data plots)
- [ECOTOX Quick User Guide](#) (2 pp, 141 K)
- [ECOTOX User Guide](#) (89 pp, 663 K)
- [ECOTOX Terms Appendix](#)

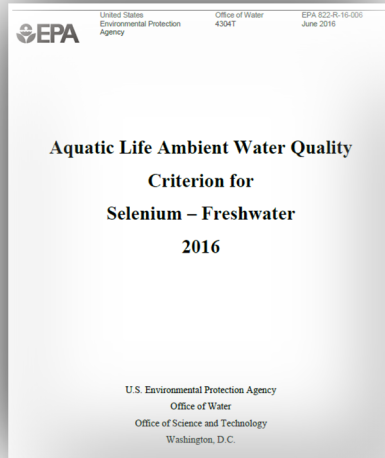
Other Links

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- [Frequent Questions](#)
- [Other Tools/Databases](#)
- [Recent Additions](#)
- [Literature Search Dates](#)

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www.epa.gov/ecotox

EPA Program and Regional Office Applications: Use in environmental decision making

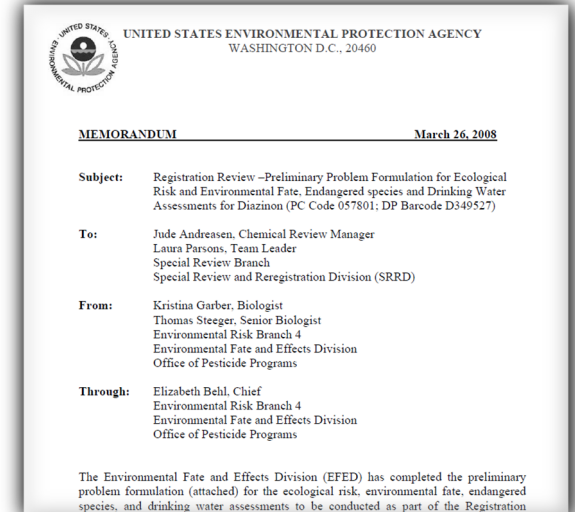
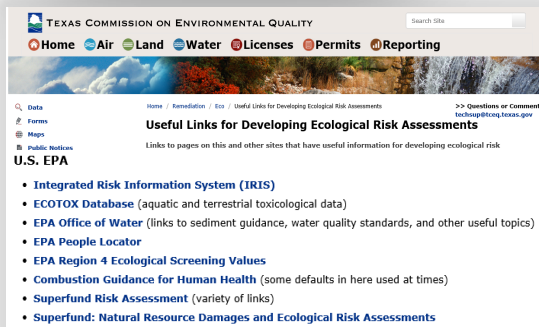


Used for every Ambient Water Quality Criteria for Aquatic Life since 1985.

Used for every Ecological Risk Assessment for Office of Pesticides for chemical registration and re-registration (FY20 – 27 chemicals).

Used by Office of Land and Emergency Management (Superfund and ORCR), HQ, Regions and States for site assessments and in emergency response.

Providing ecological hazard data for the prioritization and assessment of chemicals for TSCA/Lautenberg Act.



Overview of TSCA Work Plan Methodology

Maria Doa
U.S. EPA, Office of Pollution Prevention and Toxics
December 11, 2017



Providing ecological toxicity data for PFAS to researchers, EPA Eco Risk Assessment Forum, DoD Tri-Services ERA Work Group and others.

Ecological Hazard

Ecological hazard data are extracted from the EPA ToxValDB database where it had been compiled from the EPA ECOTOX database. Although data are available for a variety of species, only data for aquatic species are used in the current illustration. The data can come from any of the following study types: mortality:acute, mortality:chronic, reproductive:acute, reproductive:chronic, growth:acute, growth:chronic (all from ECOTOX). The types of effect levels are LDxx/LCxx/ECxx/EDxx where xx can range from 1% to 100%, and LOEL/NOEL/LOEC/NOEC. Values must be in units of mg/L. For each chemical, the lowest toxicity value was separately determined for acute and chronic studies, regardless of species. The

Applications of ECOTOX

ECOTOX Knowledgebase

*Chemical
environmental toxicity
data for aquatic life,
terrestrial plants and
wildlife*



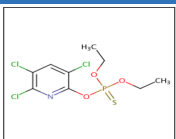
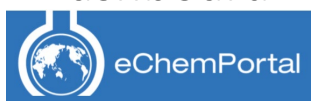
DTXSID/CASRN

Species ID; Protein ID

Integrated ontology

Reference ID

Chemicals
Dashboard



SeqAPASS



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Health &
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EPA Program Offices and Regions, States, Tribes, Other Federal Agencies and International Entities

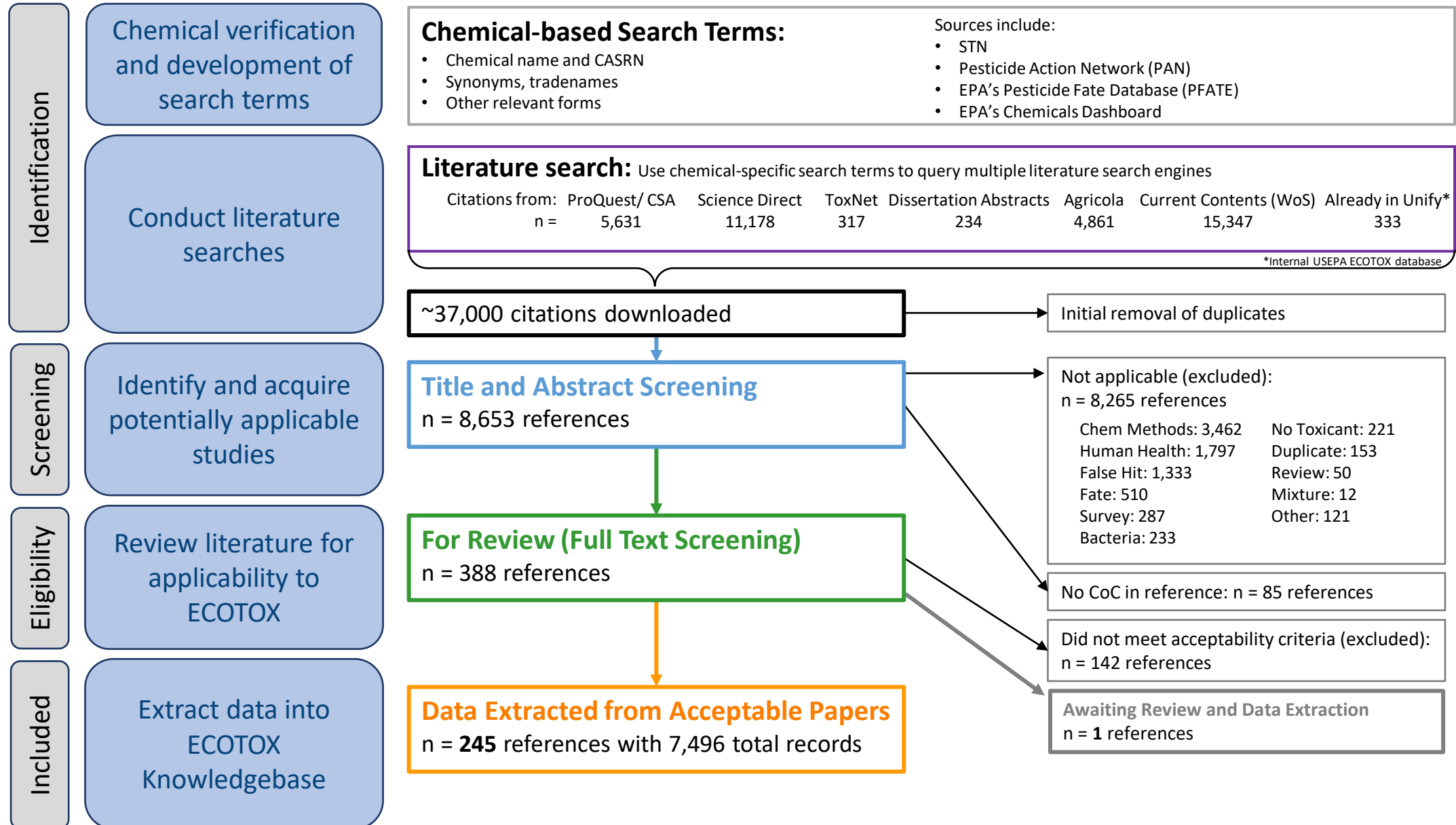
Ecological Risk Assessments
Ambient Water Quality Criteria
Ecological Screening Values
Chemical Prioritization
Emergency Response

Tools and Applications

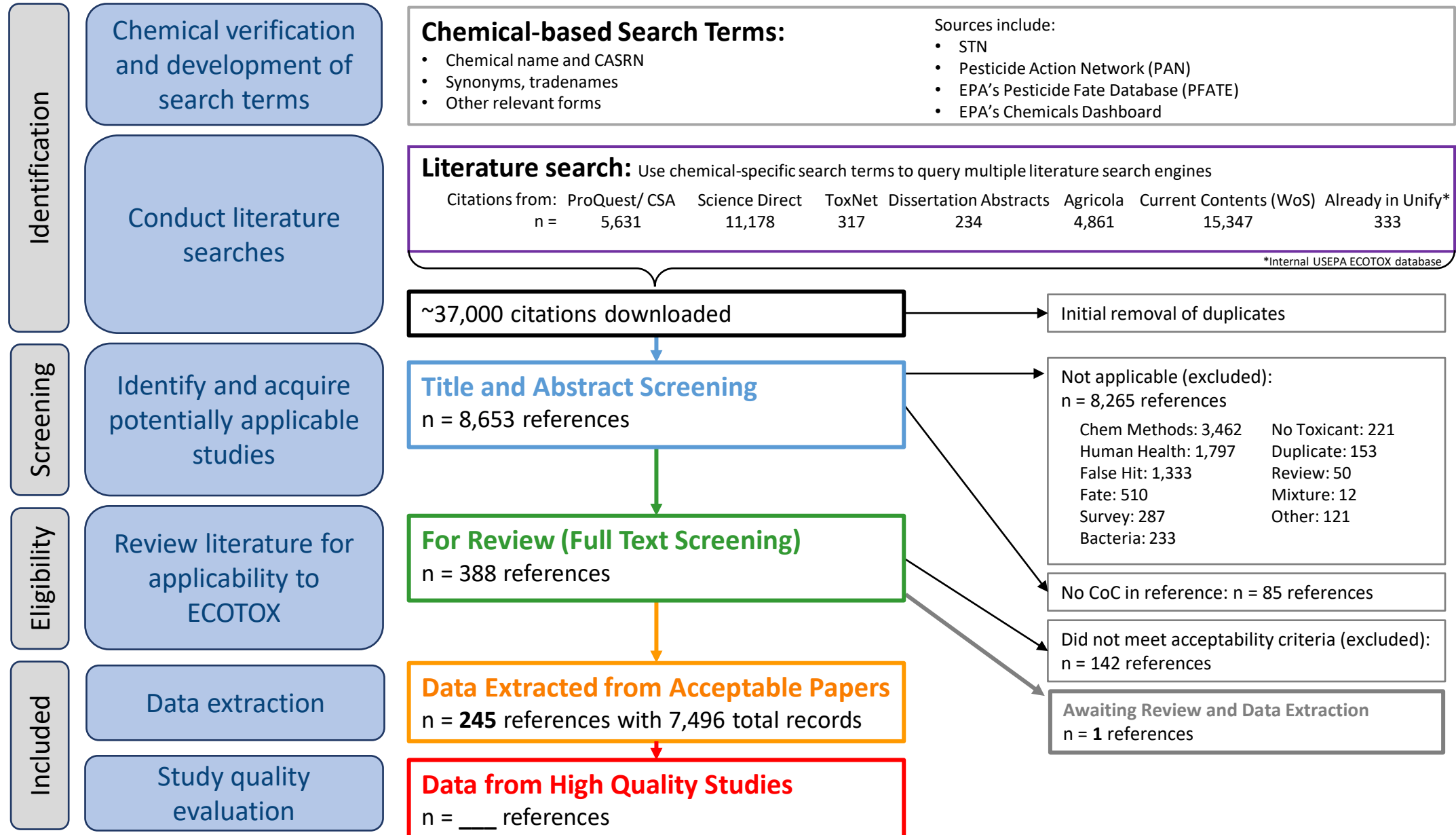
Species Sensitivity Distributions
(e.g., US EPA's WebICE, NOAA's CAFÉ)
PNECs and Eco Thresholds for Toxicological Concern
QSAR (e.g., ECOSAR, TEST, OECD QSAR Toolbox)
Bioaccumulation Factor modeling and validation
Adverse Outcome Pathway (AOP) development

**Interoperability with
databases/tools**

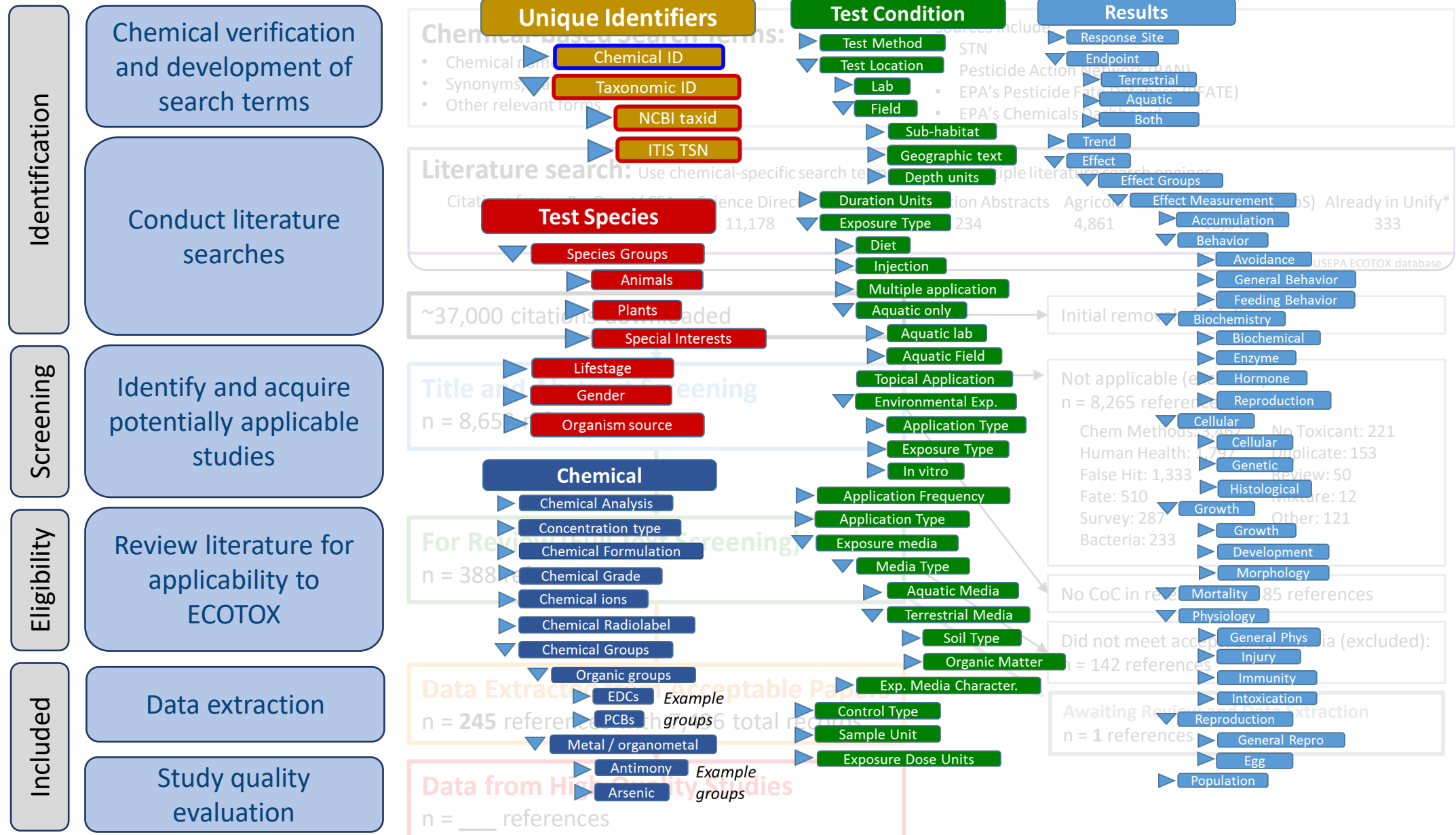
ECOTOX Pipeline: Systematic Review/Data Curation



ECOTOX Pipeline: Systematic Review/Data Curation



ECOTOX Pipeline: Systematic Review/Data Curation



ECOLOGICAL Structure-Activity Relationship Model (ECOSAR) Class Program

Ecosar Application 2.0

ECOSAR Special Cases

Organic Module

Organic

Welcome

ECOSAR Version 2.0



ECOSAR is developed and owned by the U.S. Environmental Protection Agency's Office of Chemical Safety and Pollution Prevention and is protected by copyright throughout the world. Permission is granted for individuals to download and use the software on their personal and business computers free of charge. Users may not alter, modify, merge, adapt, or prepare derivative works of the software. ECOSAR is a screening-level tool to estimate the ecological hazards of chemicals when measured data are lacking and is primarily developed for chemicals regulated under the Toxic Substances Control Act (TSCA).

Disclaimer: Experimental data sources and values estimated by EPI are not endorsed by the EPA; nor does the EPA vouch for the quality or accuracy of the data. Furthermore, professional judgement is needed to determine the applicability and accuracy of Physical/Chemical properties and fate endpoints estimated by EPI

Accept **Decline**

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<https://www.epa.gov/tsca-screening-tools/ecological-structure-activity-relationships-ecosar-predictive-model>

OPERATION MANUAL
for the
**ECOLOGICAL Structure-Activity Relationship Model
(ECOSAR)**
Class Program

**ESTIMATING TOXICITY OF INDUSTRIAL CHEMICALS TO AQUATIC
ORGANISMS USING THE
ECOSAR (ECOLOGICAL STRUCTURE ACTIVITY RELATIONSHIP) CLASS
PROGRAM**

MS-Windows Version 2.0

Contributors:

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J. Vince Nabholz^{a*}, William M. Meylan^b,
Philip H. Howard^b, and Lauren Cassidy^b

^aRisk Assessment Division (7403)
U.S. Environmental Protection Agency
1200 Pennsylvania Ave., N.W.
Washington, DC 20460
* Deceased

^bEnvironmental Health Analysis
SRC, Inc.
7502 Round Pond Road
North Syracuse, NY 13212-2558

ECOLOGICAL Structure-Activity Relationship Model (ECOSAR) Class Program

Ecosar Application 2.0

ECOSAR Special Cases

Organic Module

Organic

Organic Module

Chemical Input

CCN(CC)C(=O)C1=CC=CC(C)=C1

CAS Number: 50-00-0, 000050-00-0, 50000 SMILES: O=C

Benzamide, N,N-diethyl-3-methyl- x

Chemical Name: Benzamide, N,N-diethyl-3-methyl-

CAS: 134623

Log Kow: 2.2579

Water Solubility (mg/L): 1911.0

Melting Point (°C): -45.0

Chemical Details

SMILES: O=C(N(CC)CC)(CCCC1C)c1

MOL WT: 191.28

Log Kow: 2.2579 (estimated), 2.18 (measured)

<https://www.epa.gov/tsca-screening-tools/ecological-structure-activity-relationships-ecosar-predictive-model>

Organic Module Result Experimental Data Physical Properties K_{ow} Estimate Report

Amides

Organism	Duration	End Point	Concentration (mg/L)
Fish	96h	LC50	33.6
Daphnid	48h	LC50	31.4
Green Algae	96h	EC50	4.48
Fish		ChV	0.492
Daphnid		ChV	5.72
Green Algae		ChV	3.21
Fish (SW)	96h	LC50	33.1
Mysid (SW)	96h	LC50	2.27
Mysid (SW)		ChV	0.202
Earthworm	14d	LC50	506

Organic Module Result Experimental Data Physical Properties K_{ow} Estimate Report

Organism	Duration	End Point	Concentration (mg/L)	Reference
Fish	96h	LC50	71.2	OPP Pesticide Ecotoxicity DB
Daphnid	48h	LC50	75.0	OPP Pesticide Ecotoxicity DB
Fish	96h	LC50	110.0	DUL

Organic Module Report

Results of Organic Module Evaluation

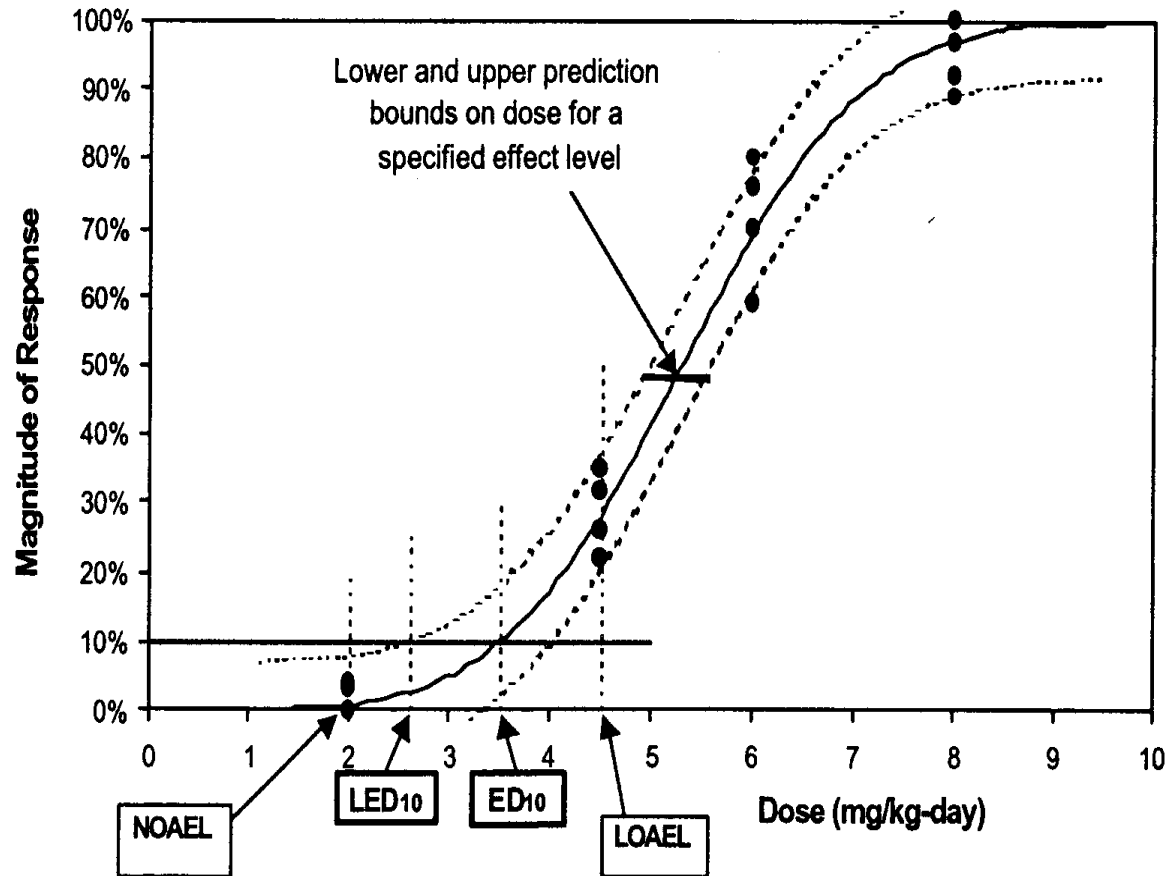
CAS	Name	SMILES
134623	Benzamide, N,N-diethyl-3-methyl-	<chem>O=C(N(CC)CC)(CCCC1C)c1</chem>

Structure

Details

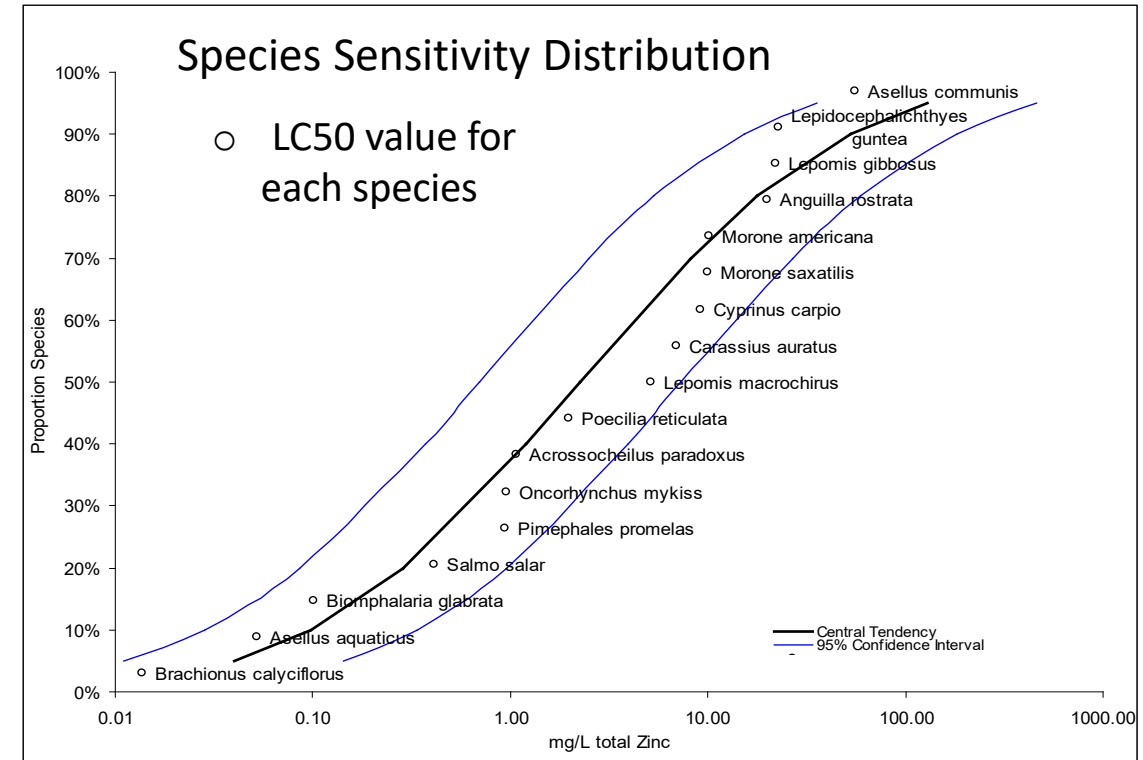
Mol Wt	191.28
Selected LogKow	2.26
Selected Water Solubility (mg/L)	1910.97
Selected Melting Point (°C)	-45
Estimated LogKow	2.26
Estimated Water Solubility (mg/L)	1910.97
Measured LogKow	2.18
Measured Water Solubility (mg/L)	1911.0
Measured Melting Point (°C)	-45

Hazard: Individual Species



Hazard: Multiple Species

Increasing proportion
of species affected (LC_{50})



Increasing stressor intensity

Species Sensitivity Distribution Toolbox

<https://www.epa.gov/chemical-research/species-sensitivity-distribution-ssd-toolbox>

EPA/600/R-18/116

User's Manual: SSD Toolbox Version 1.0

SSD Toolbox

File Plot

No data imported

Fit Distribution

Distribution:
normal

Fitting method
maximum likelihood

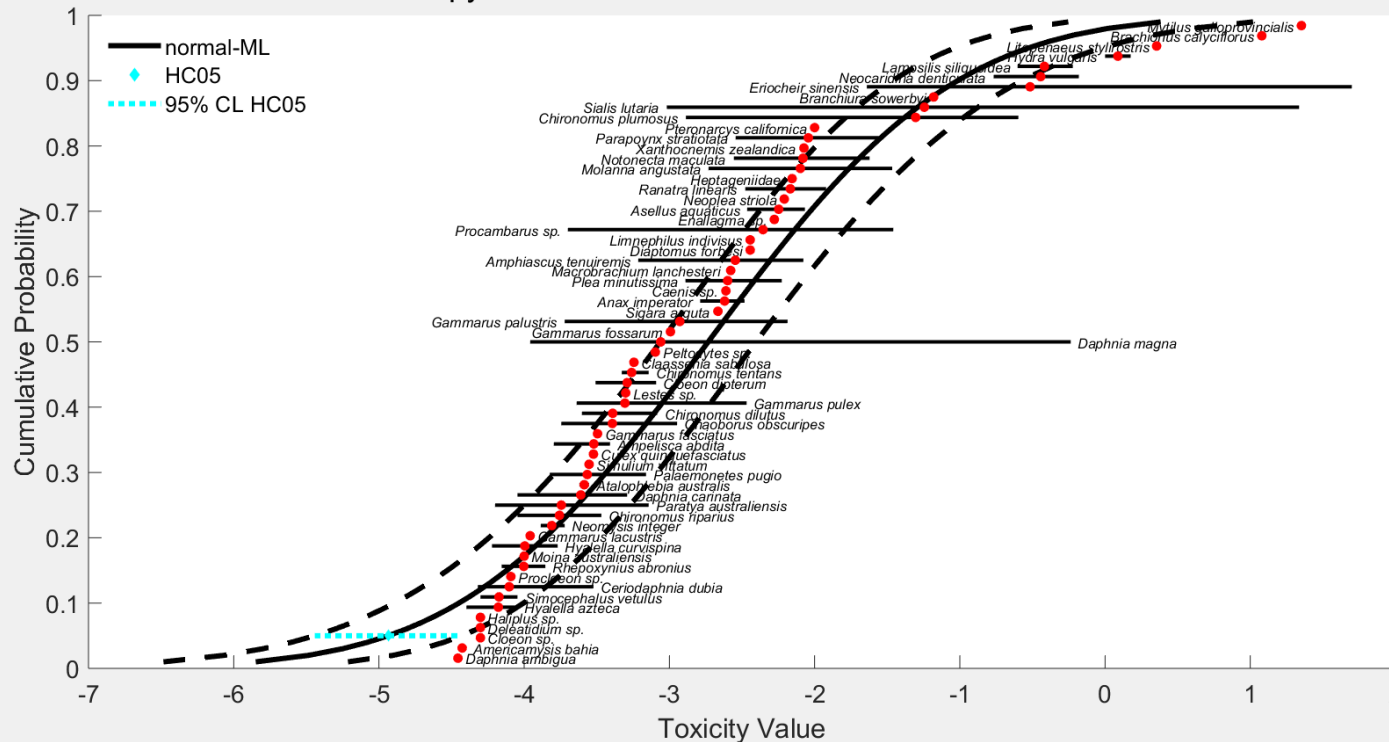
Goodness of Fit:
Iterations: 1000

Scaling parameters
☐ Scale to Body Weight
Scaling factor: 1.15
Target weight: 100 g

Status:
Ready

Results:

Chlorpyrifos Inverts MortLC50 ImmbEC50 - SSD = Y



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2020

Data Sources and Tools

- CompTox Chemicals Dashboard – A ‘first-stop-shop’ for chemical information.
<https://comptox.epa.gov/dashboard>
 - Chemical Properties, Structure
 - Toxicity
 - Bioactivity
 - Exposure
 - Predictions
 - Links
- ToxRefDB (version 2) – Toxicity results from >5,000 in vivo studies, conducted largely to guidelines or specifications from the US EPA and National Toxicology Program.
<https://doi.org/10.1016/j.reprotox.2019.07.012>
- ECOTOX Knowledgebase – Single chemical environmental toxicity data on aquatic life, terrestrial plants and wildlife. <https://cfpub.epa.gov/ecotox/>
- InVitroDB – ToxCast data from assays testing chemical activity. <https://www.epa.gov/chemical-research/exploring-toxcast-data>
- CPDat (Chemical and Products Database) – Information mapping more than 49,000 chemicals to usage or function in 16,000 consumer products. <https://www.epa.gov/chemical-research/chemical-and-products-database-cpdat>

Data Sources and Tools

- Read-Across and Quantitative Structure Activity Relationship models
 - OPERA (Open Structure-activity/property Relationship App) – Provide predictions of physicochemical properties and chemical activity to non-animal approaches for predicting toxicity. <https://ntp.niehs.nih.gov/whatwestudy/niceatm/comptox/ct-opera/opera.html>
 - ECOSAR (Ecological Structure Activity Relationships) – Providing predictions of acute and chronic toxicity to aquatic organisms. <https://www.epa.gov/tsca-screening-tools/ecological-structure-activity-relationships-ecosar-predictive-model>
 - TEST (Toxicity Estimation Software Tool) – Provide estimates of toxicity of chemicals using QSARs. <https://www.epa.gov/chemical-research/toxicity-estimation-software-tool-test>
- htk (High-Throughput Toxicokinetics) R Package – Includes models and databases to help researchers, risk assessors, and regulators understand how chemicals interact with the body. <https://cran.r-project.org/web/packages/htk/index.html>
- SSD Toolbox (Species Sensitivity Distribution Toolbox) – Simplifies the process of generating Species Sensitivity Distributions by gathering a variety of algorithms to support users in fitting, summarizing, visualizing and interpreting SSDs. <https://www.epa.gov/chemical-research/species-sensitivity-distribution-ssd-toolbox>
- McNest (Markov Chain Nest Productivity Model) – Predicts annual reproductive success of bird populations based on existing toxicity and species life history information. <https://www.epa.gov/chemical-research/markov-chain-nest-productivity-model>
- Fish Toxicity Translator – A mechanistic population model to estimate population-level effects of chemical exposure scenarios based on existing toxicity and life history characteristics on fish.
- SeqAPASS (Sequence Alignment to Predict Across Species Susceptibility) – Provides online screening tool to extrapolate toxicity information across species based on protein targets. <https://seqapass.epa.gov/seqapass/>
- AOPwiki – An Adverse Outcome Pathway (AOP) is a structured representation of biological events leading to adverse effect(s). The AOPwiki is a repository for AOPs developed and in development. <https://aopwiki.org/>