

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

Jennifer Olker  
[olker.jennifer@epa.gov](mailto:olker.jennifer@epa.gov)

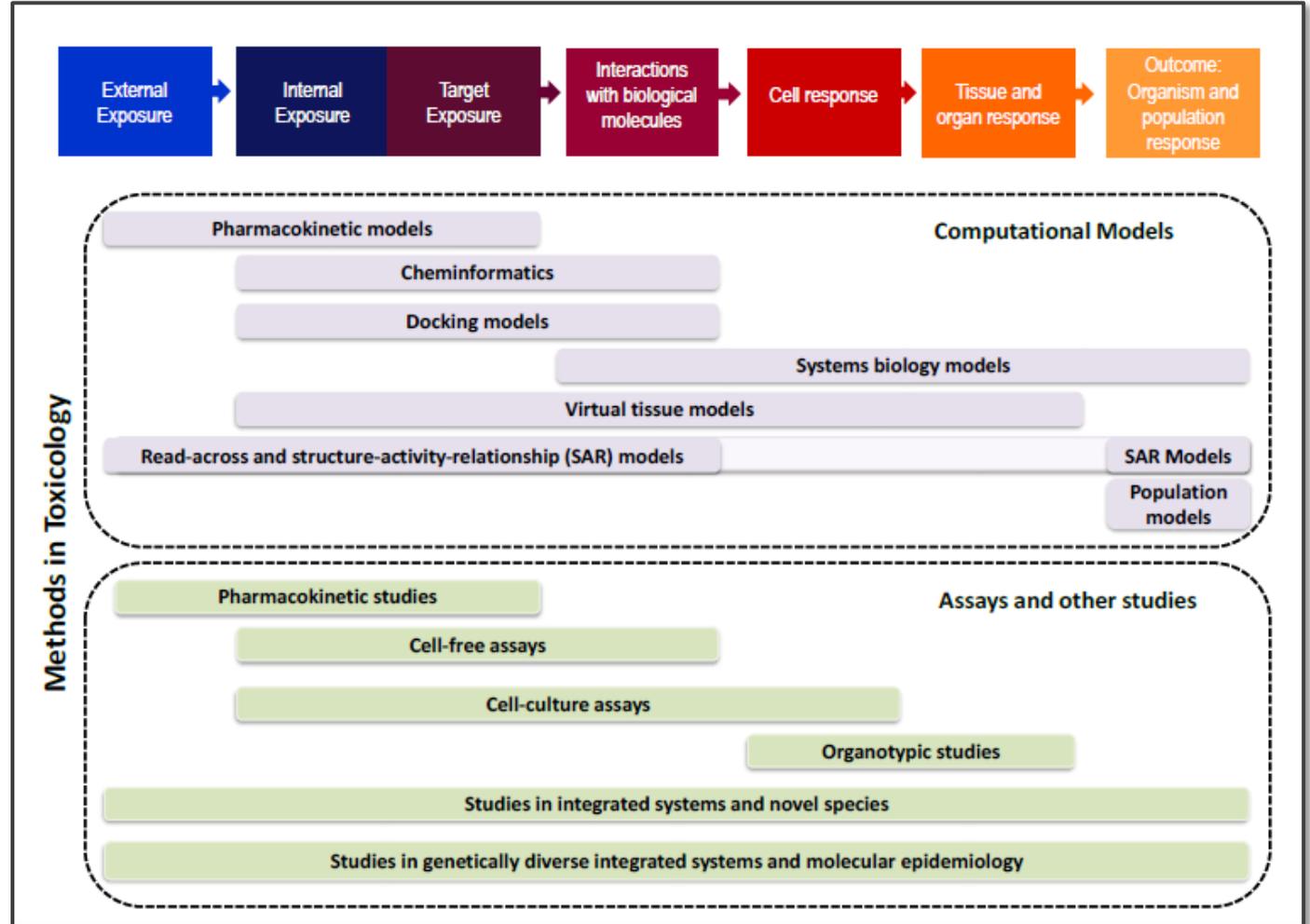
*Center for Computational Toxicology & Exposure  
US EPA Office of Research and Development (ORD)*

**Georgetown University  
EMAP Program  
April 2021**

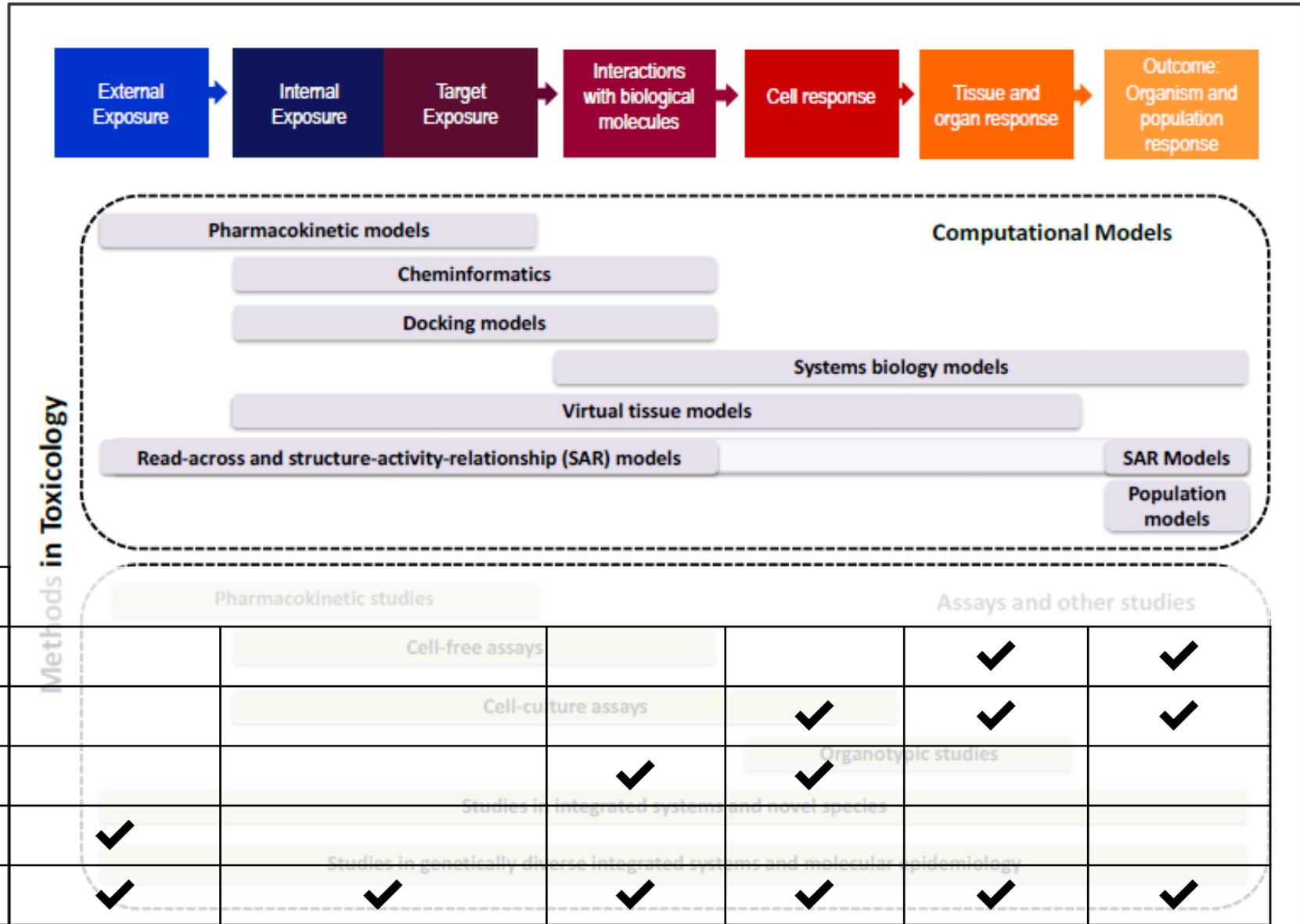
# Toxicology Moving to Embrace 21<sup>st</sup> Century Methods



<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

Source	External Exposure	Internal Exposure	Target Exposure	Interactions with biological molecules	Cell response	Tissue and organ response	Outcome: Organism and population response
<b>CompTox Chemicals Dashboard</b>	✓	Pharmacokinetic models	✓	✓	✓	Computational Models	✓
httk	✓	Cheminformatics	✓				
OPERA	✓	Docking models			Systems biology models		
<b>SSD Toolbox</b>				Virtual tissue models			✓
<b>EcoSAR</b>		Read-across and structure-activity-relationship (SAR) models					SAR Models
<b>McNest</b>							Population models
<b>Toxicity Translators</b>		Pharmacokinetic studies				Assays and other studies	✓
ToxRefDB		Cell-free assays				✓	✓
<b>ECOTOX KB</b>		Cell-culture assays			✓	✓	✓
<b>InVitro DB</b>				✓	Organotypic studies		
CPDat	✓			Studies in integrated systems and novel species			
Open Literature	✓		✓	Studies in genetically diverse integrated systems and molecular epidemiology	✓	✓	✓

Methods in Toxicology

Multiple Species

Populations

Multiple Species

# CompTox Chemicals Dashboard

https://comptox.epa.gov/dashboard



## CompTox Chemicals Dashboard

883 Thousand Chemicals

Window Snip

Chemicals

Product/Use Categories

Assay/Gene

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.](#)

# CompTox Chemicals Dashboard

https://comptox.epa.gov/dashboard


 United States Environmental Protection Agency
 

[Home](#)
[Advanced Search](#)
[Batch Search](#)
[Lists](#)
[Predictions](#)
[Downloads](#)

## CompTox Chemicals Dashboard

883 Thousand Chemicals

Chemicals | Product/Use Categories | Assay/Gene

Search for chemical by system

Identifier substring search

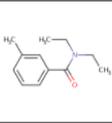

United States Environmental Protection Agency

Copy Share Submit Comment

**New article to help u**

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

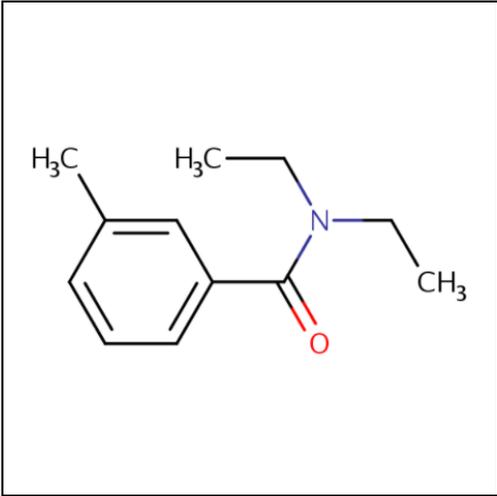
A new article regarding the batch Enabling High-Throughput Search



### DEET

134-62-3 | DTXSID2021995

Searched by DSSTox Substance Id.



**DETAILS**

- EXECUTIVE SUMMARY
- PROPERTIES
- ENV. FATE/TRANSPORT
- HAZARD
- ▶ SAFETY
- ▶ ADME
- ▶ EXPOSURE
- ▶ BIOACTIVITY
- SIMILAR COMPOUNDS
- GENRA (BETA)
- RELATED SUBSTANCES
- SYNONYMS
- ▶ LITERATURE
- LINKS

**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:** C<sub>12</sub>H<sub>17</sub>NO  Mol File  Find All Chemicals

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

 **Monoisotopic Mass:** 191.131014 g/mol

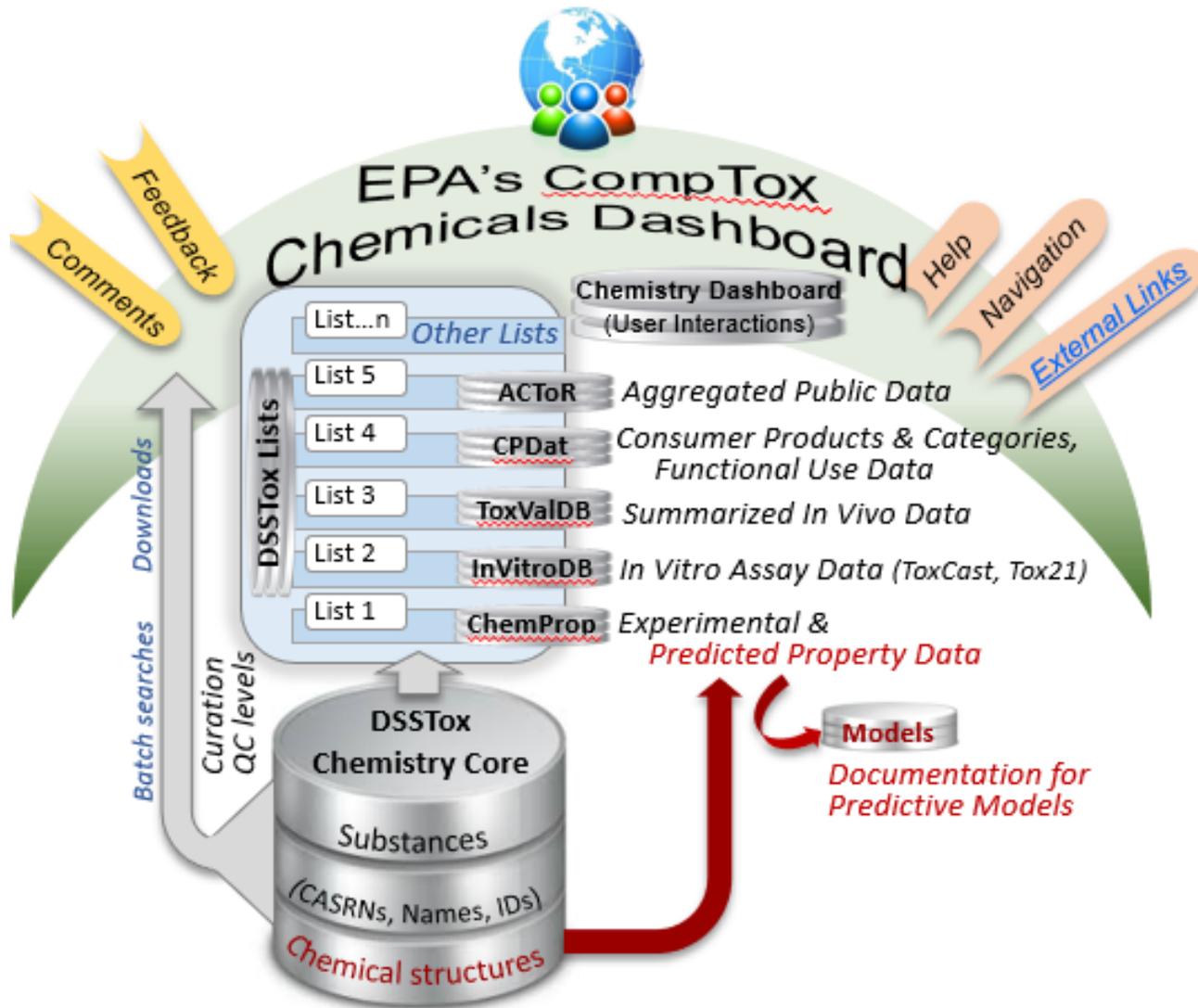
**Structural Identifiers**

**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

CompTox Chemicals Dashboard

SEARCH

883 Thousand Chemicals



Chemicals Product/Use Categories Assay/Gene

Search for chemical by system  
 Identifier substring search

Copy Share Submit Comment Search all data

## New article to help u

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

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

### DETAILS

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BIOACTIVITY

SIMILAR COMPOUNDS

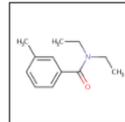
GENRA (BETA)

RELATED SUBSTANCES

SYNONYMS

LITERATURE

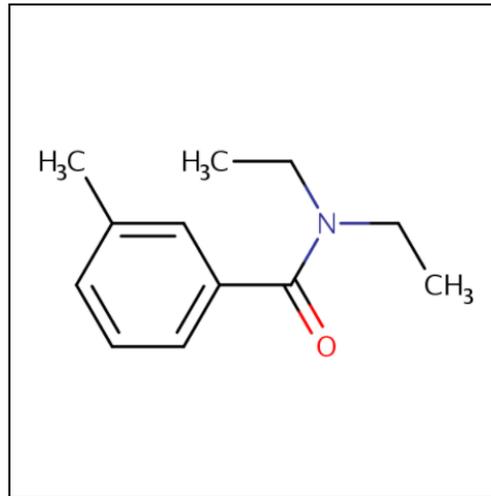
LINKS



DEET

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:** C<sub>12</sub>H<sub>17</sub>NO [Mol File](#) [Find All Chemicals](#)  
**Average Mass:** 191.274 g/mol [Isotope Mass Distribution](#)  
**Monoisotopic Mass:** 191.131014 g/mol

### Structural Identifiers

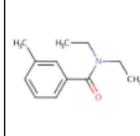
### Linked Substances

### Presence in Lists

### Record Information

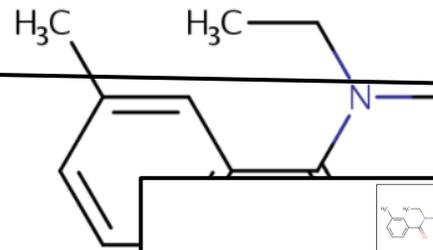
# CompTox Chemicals Dashboard

https://comptox.epa.gov/dashboard



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

- DETAILS**
- EXECUTIVE SUMMARY
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**DEET**  
134-62-3 | DTXSID2021995  
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



**DEET**  
134-62-3 | DTXSID2021995  
Searched by DSSTox Substance Id.

Hazard

Human Eco



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

Chemical Activity Summary

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



**DEET**  
134-62-3 | DTXSID2021995  
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

BIOACTIVITY

ASSAY DETAILS

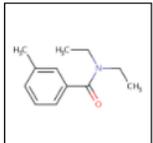
AC50 (µM): 0.10  
Scaled top: 1.08  
Assay Endpoint Name: LFEA\_HepaRG\_GADD45G\_up  
Gene Symbol: GADD45G  
Organism: human  
Tissue: liver  
Assay Format Type: cell-based  
Biological Process Target: regulation of transcription factor activity  
Detection Technology: Fluidigm qRT-PCR  
Analysis Direction: positive  
Intended Target Family: mutagenicity response  
Description: Change in transcription factor expression relative to control (delta-delta-cf) 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

https://comptox.epa.gov/dashboard


United States Environmental Protection Agency
Home [Advanced Search](#) [Batch Search](#) [Lists](#) [Predictions](#)

**DEET**  
134-62-3 | DTXSID2021995  
Searched by DSSTox Substance Id.



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- HAZARD
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- BIOACTIVITY
- SIMILAR COMPOUNDS**
- GENRA (BETA)
- RELATED SUBSTANCES
- SYNONYMS
- LITERATURE
- LINKS

**DEET**  
134-62-3 | DTXSID2021995  
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DETAILS

EXECUTIVE SUMMARY

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HAZARD

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BIOACTIVITY

**SIMILAR COMPOUNDS**

GENRA (BETA)

RELATED SUBSTANCES

SYNONYMS

LITERATURE

LINKS

**SIMILARITY**

Searched with a similarity threshold of 0.8

607 chemicals

Select all Download Send to Batch Search Similarity DTXSID CASRN TOXCAST Similarity Hide chemicals that are: Filter by Name or CASRN



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

DETAILS

EXECUTIVE SUMMARY

PROPERTIES

ENV. FATE/TRANSPORT

HAZARD

SAFETY

ADME

**LITERATURE**

Abstract Sifter

1416 of 1416 articles loaded...

Optionally, edit the query before retrieving.

1) Select PubMed starting point query then 2) click on Retrieve.

Select a Query Term Retrieve Articles

To find articles quickly, enter terms to sift abstracts.

Download / Send to... Download Sifter for Excel

PMID	Year	Title	Authors	Journal	Rev
11111	2010	Regulatory toxicology and pharmacology	Harada, J.	Regulatory toxicology and pharmacology : RTP	
11112	2010	Journal of medical entomology	Batter, O'Dell; Syed, Wheeler; Debb.	Journal of medical entomology	
11113	2010	Journal of Ayub Medical College, Abbottabad : JAMC	Nadeem, Ali; Ahmad, Anwar; Mustaf.	Journal of Ayub Medical College, Abbottabad : JAMC	
11114	2010	Journal of hazardous materials	vic	Journal of hazardous materials	
11115	2010	The Science of the total environment	Fildier, Libert; Giroud; Hammada; H.	The Science of the total environment	
11116	2010	Parasites & vectors	ada; Kuramoto; Mitsuhashi; Saitoh...	Parasites & vectors	
11117	2010	Journal of environmental science and health. Part ...	Shao; He; Zhang; Jia	Journal of environmental science and health. Part ...	
11118	2010	The Science of the total environment	Jankowski; Ferrey; Chenuaux-Ibrahi.	The Science of the total environment	
11119	2010	Current biology : CB	enas; Afify; Yilmaz; Potter; Laminett...	Current biology : CB	
11120	2010	Journal of the American Mosquito Control Association	nte; Cuba; Allen; Becnet; Linthicum	Journal of the American Mosquito Control Association	
11121	2010	Journal of the American Mosquito Control Association	ffe; MacKenzie	Journal of the American Mosquito Control Association	
11122	2010	The Journal of dermatology		The Journal of dermatology	✓
11123	2010	Materials (Basel, Switzerland)	g; Focke; Boldt; Androsch; Leuteritz	Materials (Basel, Switzerland)	

**LINKS**

General

- EPA Substance Registry Service
- PubChem
- Chempidder
- 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
- CaIEPA OEHHA
- NIOSH IDLH Values
- LactMed
- ECOTOX

Publications

- Toxline
- PPRTWWEB
- 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
- LSDER

# CompTox Chemicals Dashboard

https://comptox.epa.gov/dashboard

## Select List

Download Columns 10

Search query Copy 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 (-NH <sub>2</sub> ) 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 << < 1 2 3 4 5 6 7 8 9 10 > >> Last

Showing 1 to 10 of 297 records

- Library (Phase II Subset)
- TOXCAST: EPA ToxCast Screening Library
- OCRINE: EDSP Universe of Chemicals
- B: National Environmental Methods Index
- ToxCast Screening Assay In Vitro DB Version 3
- Library
- ion (updated March 20th 2020).

LITERATURE

LINKS

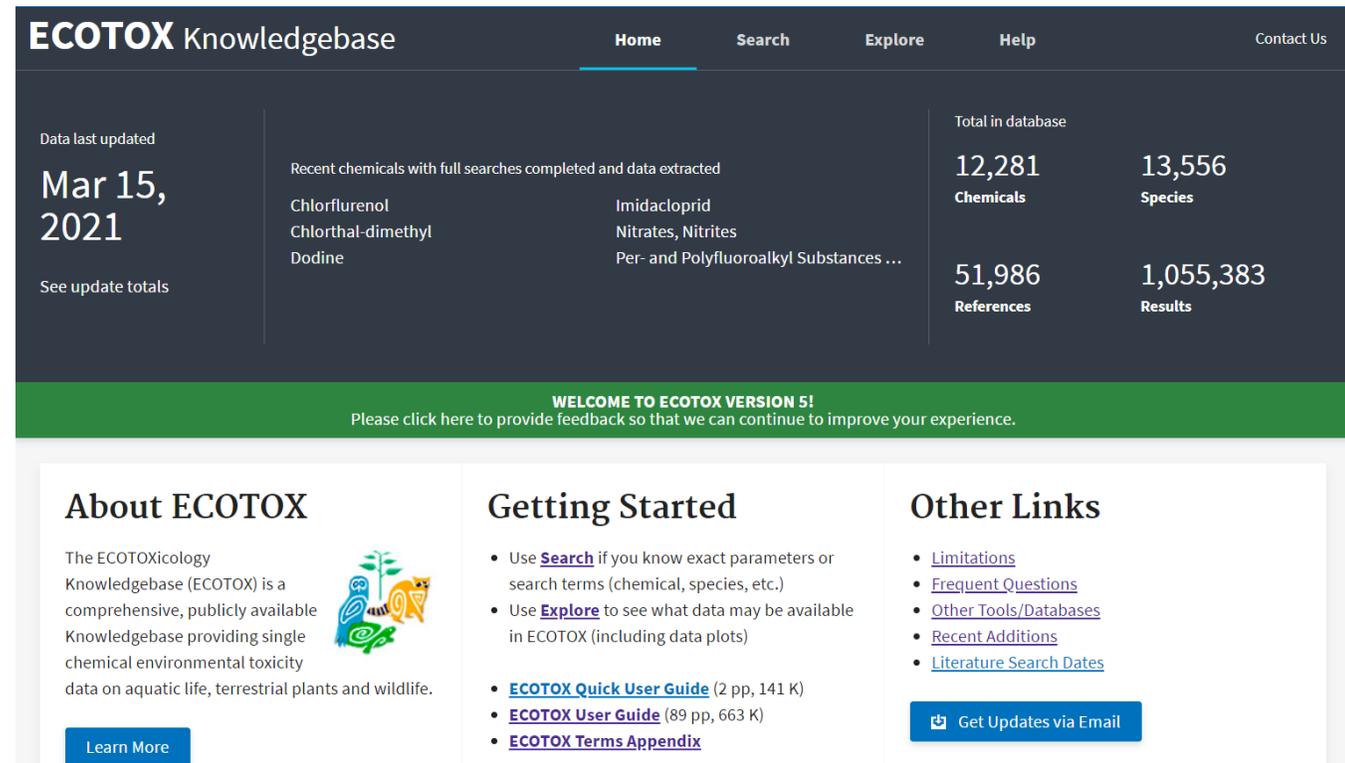
Other

- LIST: BLOODEXPOSOME
- CATEGORY|COSMETICS: COSMOS DB cosmetics database
- EPA|LIST: Article "Workflow for Defining Reference Chemicals for Assessing Performance of In Vitro Assays"
- LIST: Chemicals in biosolids
- NORMAN: REACH Chemicals List Provided to NORMAN Network
- MASSSPEC: CASMI2016 Training dataset
- NORMAN: 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



The screenshot shows the ECOTOX Knowledgebase website. At the top, there is a navigation bar with links for Home, Search, Explore, Help, and Contact Us. Below the navigation bar, the page is divided into several sections:

- Data last updated:** Mar 15, 2021. A link to "See update totals" is provided.
- Recent chemicals with full searches completed and data extracted:**
  - Chlorflurenol
  - Chlorthal-dimethyl
  - Dodine
  - Imidacloprid
  - Nitrates, Nitrites
  - Per- and Polyfluoroalkyl Substances ...
- Total in database:**

12,281	13,556
Chemicals	Species
51,986	1,055,383
References	Results

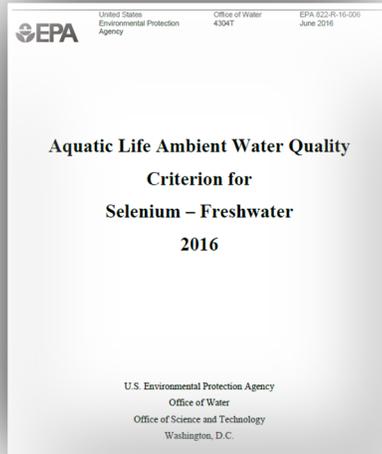
A green banner below the statistics reads: "WELCOME TO ECOTOX VERSION 5! Please click here to provide feedback so that we can continue to improve your experience."

The main content area is divided into three columns:

- About ECOTOX:** Describes the ECOTOXicology Knowledgebase (ECOTOX) as a comprehensive, publicly available Knowledgebase providing single chemical environmental toxicity data on aquatic life, terrestrial plants and wildlife. Includes a "Learn More" button and an illustration of a bird, a tree, and a fish.
- Getting Started:** Lists instructions on how to use the site (Search, Explore) and provides links to the ECOTOX Quick User Guide (2 pp, 141 K), ECOTOX User Guide (89 pp, 663 K), and ECOTOX Terms Appendix.
- Other Links:** Lists links for Limitations, Frequent Questions, Other Tools/Databases, Recent Additions, and Literature Search Dates. Includes a "Get Updates via Email" button.

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

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



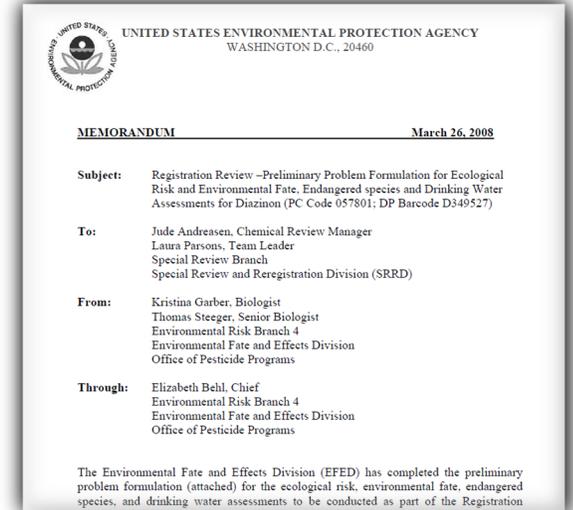
*Used for every Ambient Water Quality Criteria for Aquatic Life since 1985.*

*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.*

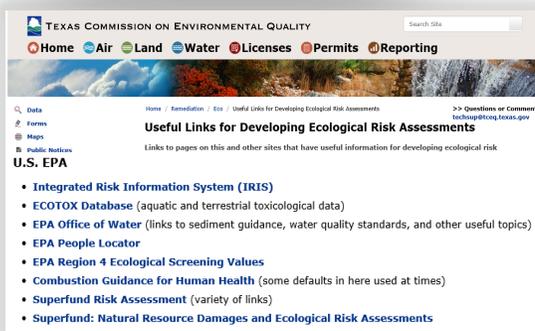
*Providing ecological hazard data for the prioritization and assessment of chemicals for TSCA/Lautenberg Act.*

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



## Overview of TSCA Work Plan Methodology

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



### 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*



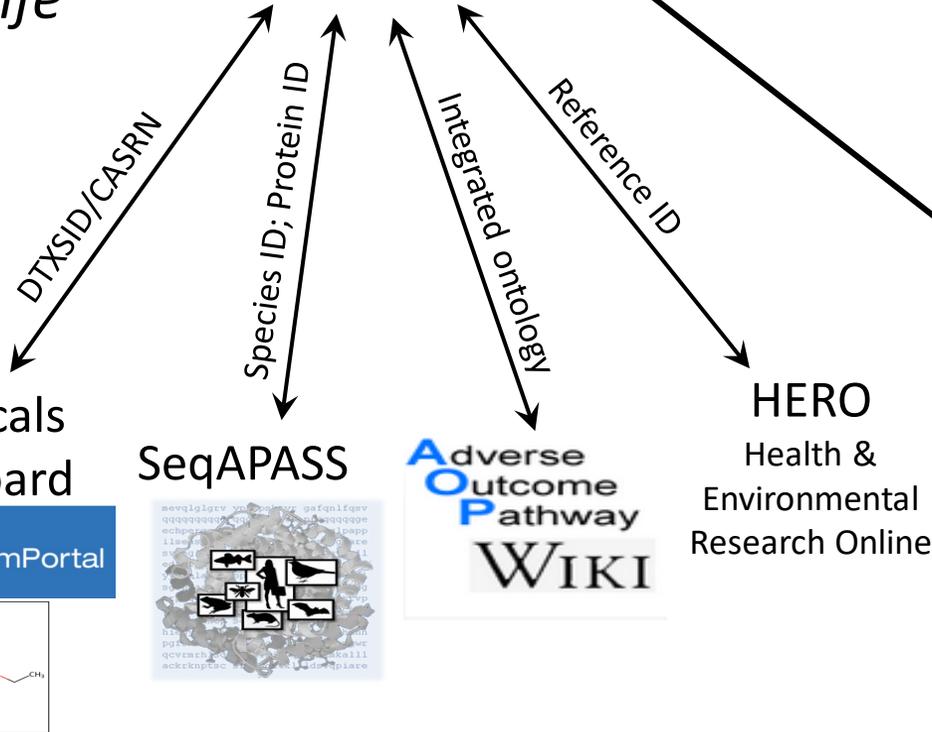
## EPA Program Offices and Regions, States, Tribes, Other Federal Agencies and International Entities

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

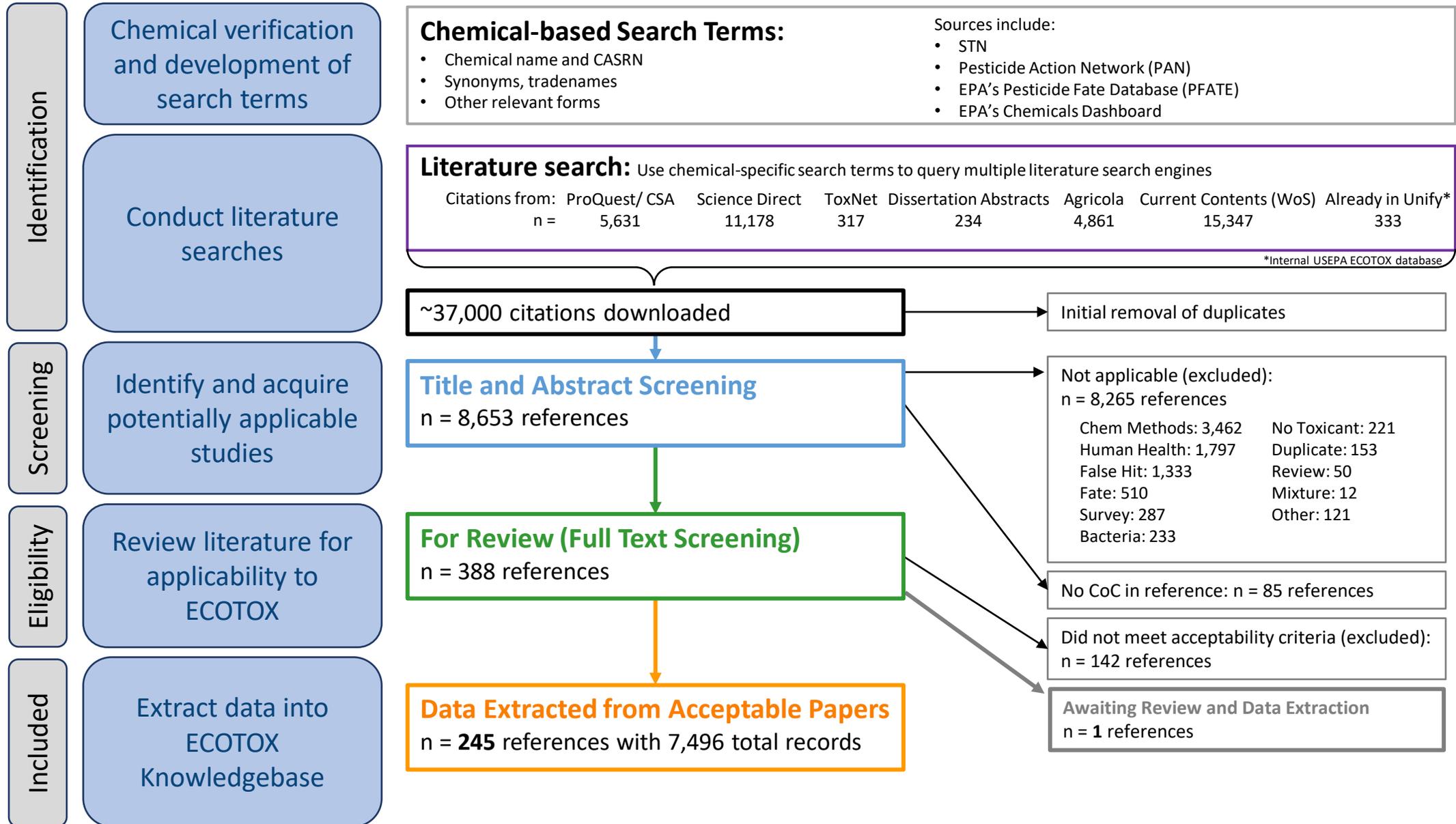
## Tools and Applications

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

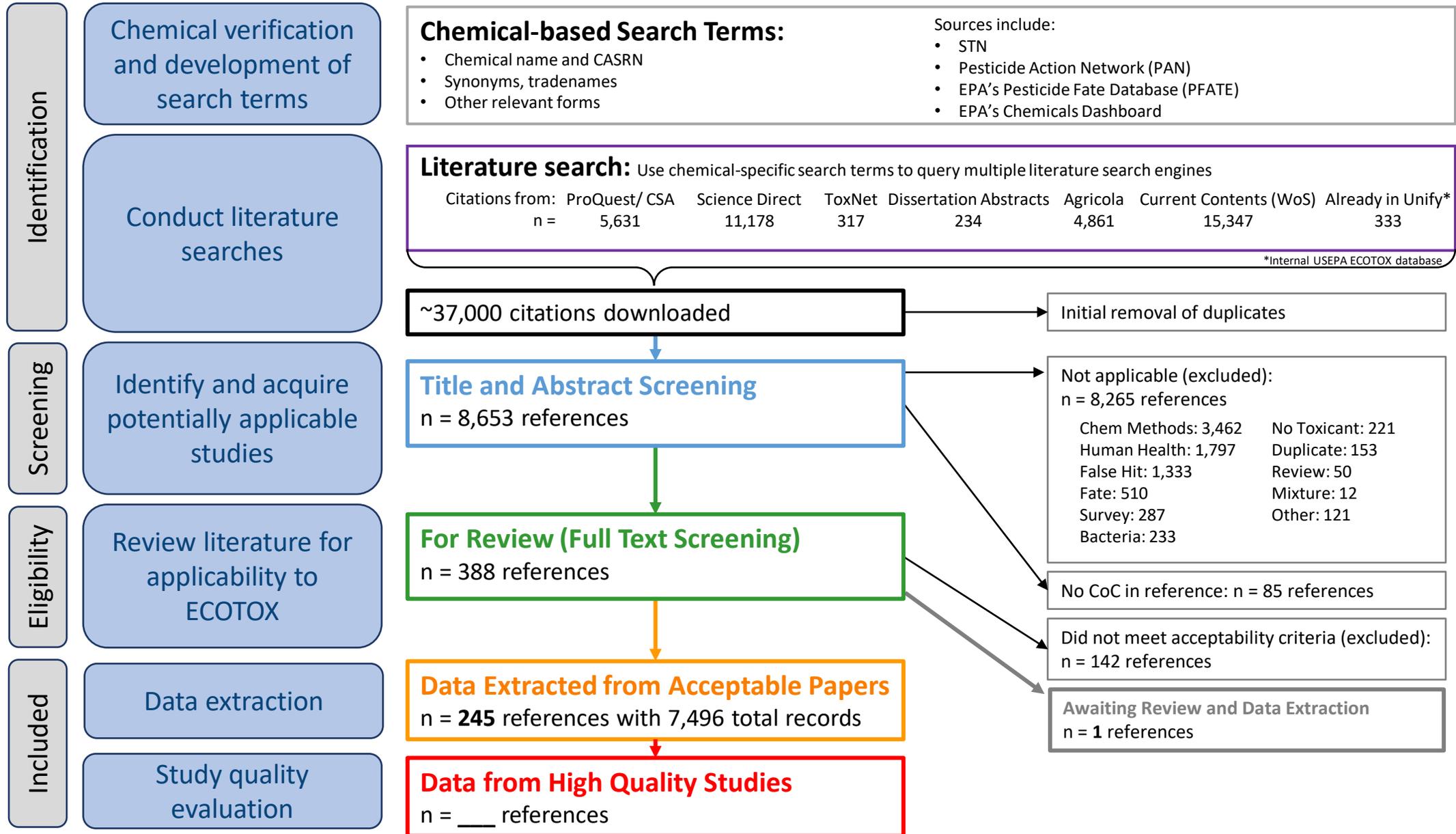
**Interoperability with databases/tools**



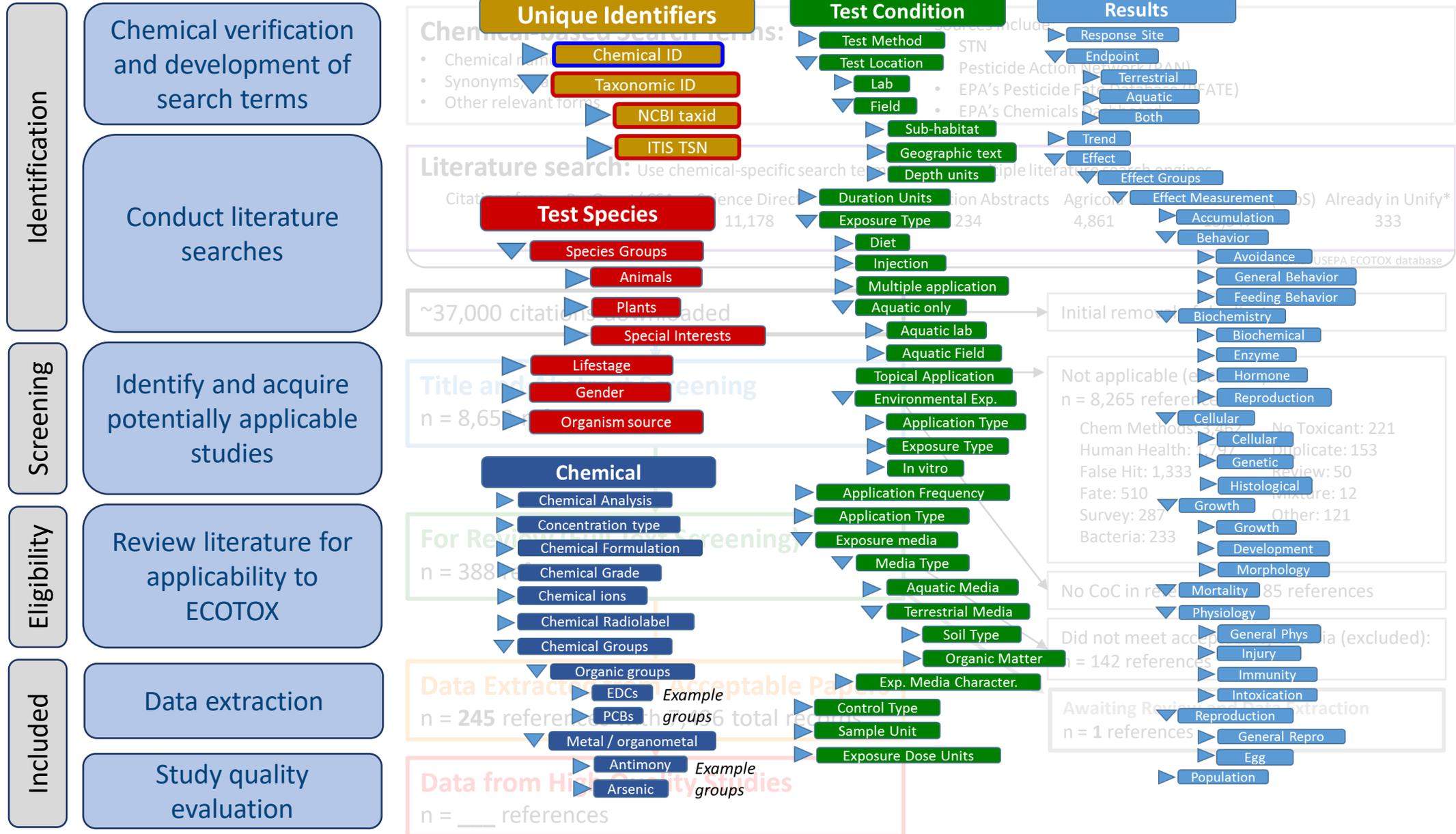
# ECOTOX Pipeline: Systematic Review/Data Curation



# ECOTOX Pipeline: Systematic Review/Data Curation



# ECOTOX Pipeline: Systematic Review/Data Curation



# ECOLOGICAL Structure-Activity Relationship Model (ECOSAR) Class Program

Ecosar Application 2.0

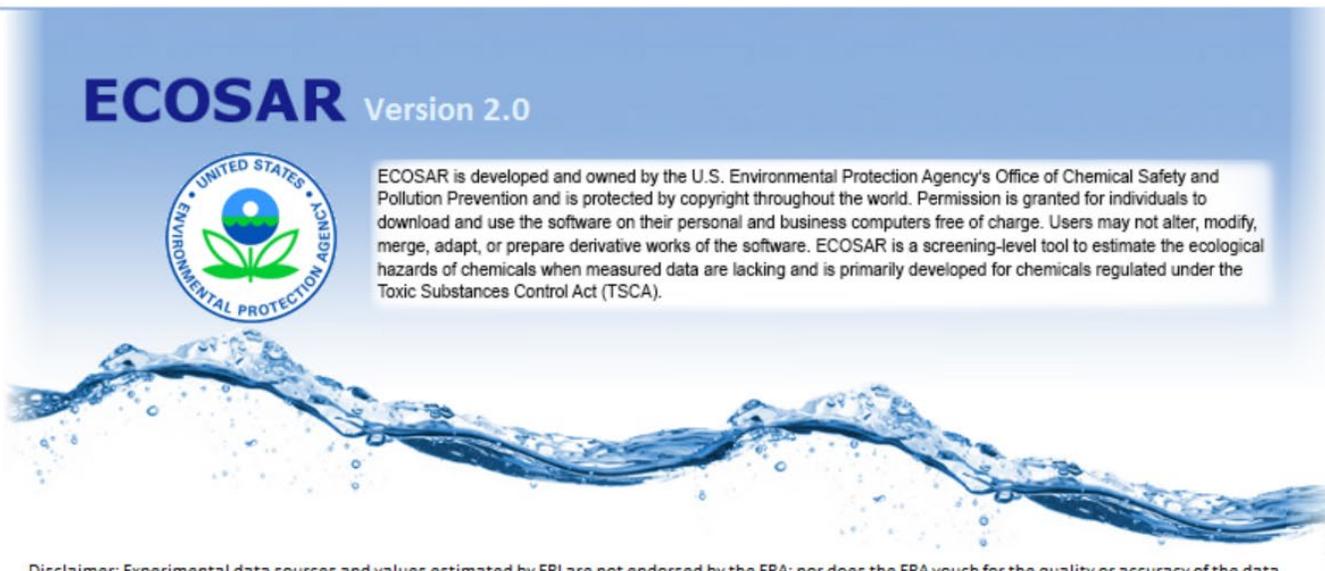
ECOSAR Special Cases

Organic Module

Organic

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

Welcome



**ECOSAR** Version 2.0



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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

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**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:  
Kelly Mayo-Bean<sup>a</sup>, Kendra Moran-Bruce<sup>a</sup>,  
J. Vince Nabholz<sup>a</sup>, William M. Meylan<sup>b</sup>,  
Philip H. Howard<sup>b</sup>, and Lauren Cassidy<sup>b</sup>

<sup>a</sup>Risk Assessment Division (7403)  
U.S. Environmental Protection Agency  
1200 Pennsylvania Ave., N.W.  
Washington, DC 20460  
\* Deceased

<sup>b</sup>Environmental Health Analysis  
SRC, Inc.  
7502 Round Pond Road  
North Syracuse, NY 13212-2558

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# ECOLOGICAL Structure-Activity Relationship Model (ECOSAR) Class Program

Ecocar 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-

**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)c(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<sub>ow</sub> 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<sub>ow</sub> 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

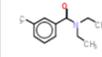
Created on Apr 25, 2021 4:26:34 PM

## Organic Module Report

Results of Organic Module Evaluation

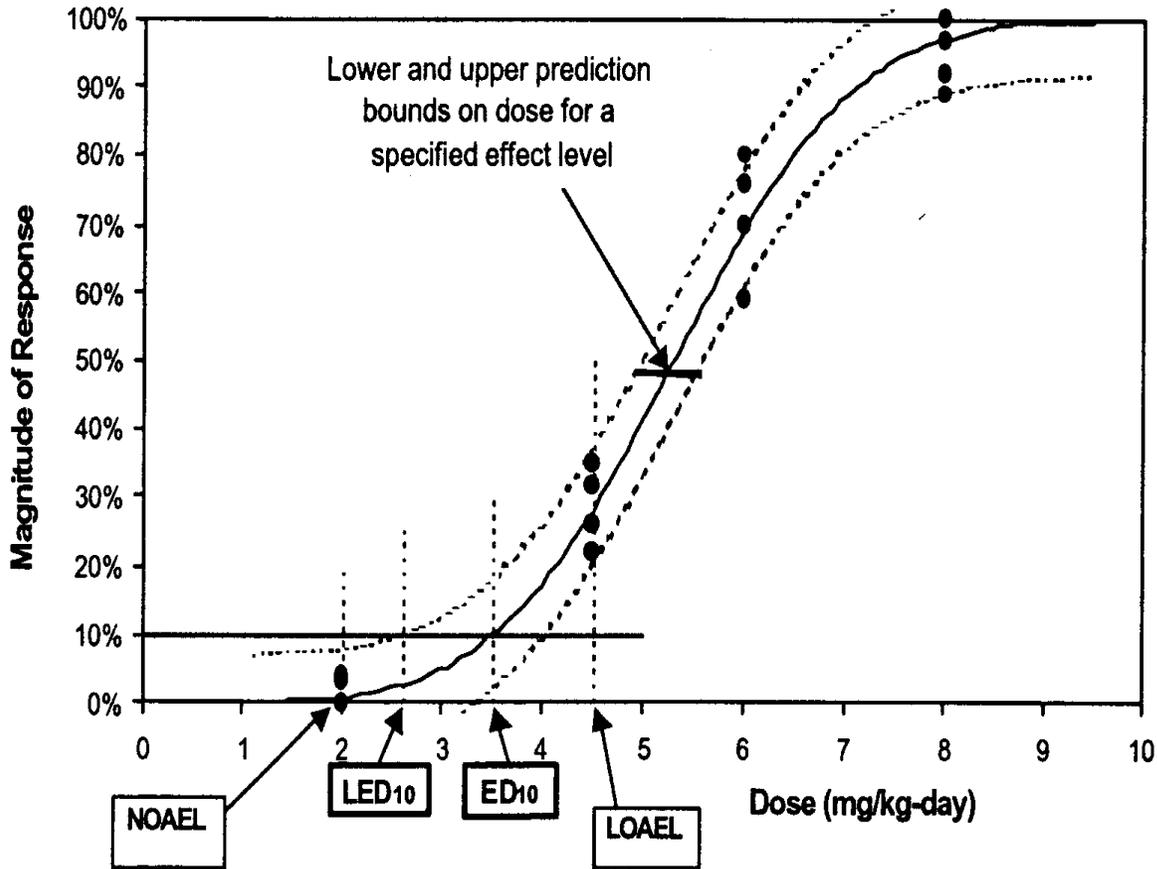
CAS	Name	SMILES
134623	Benzamide, N,N-diethyl-3-methyl-	O=C(N(CC)CC)c(cccc1C)c1

Structure



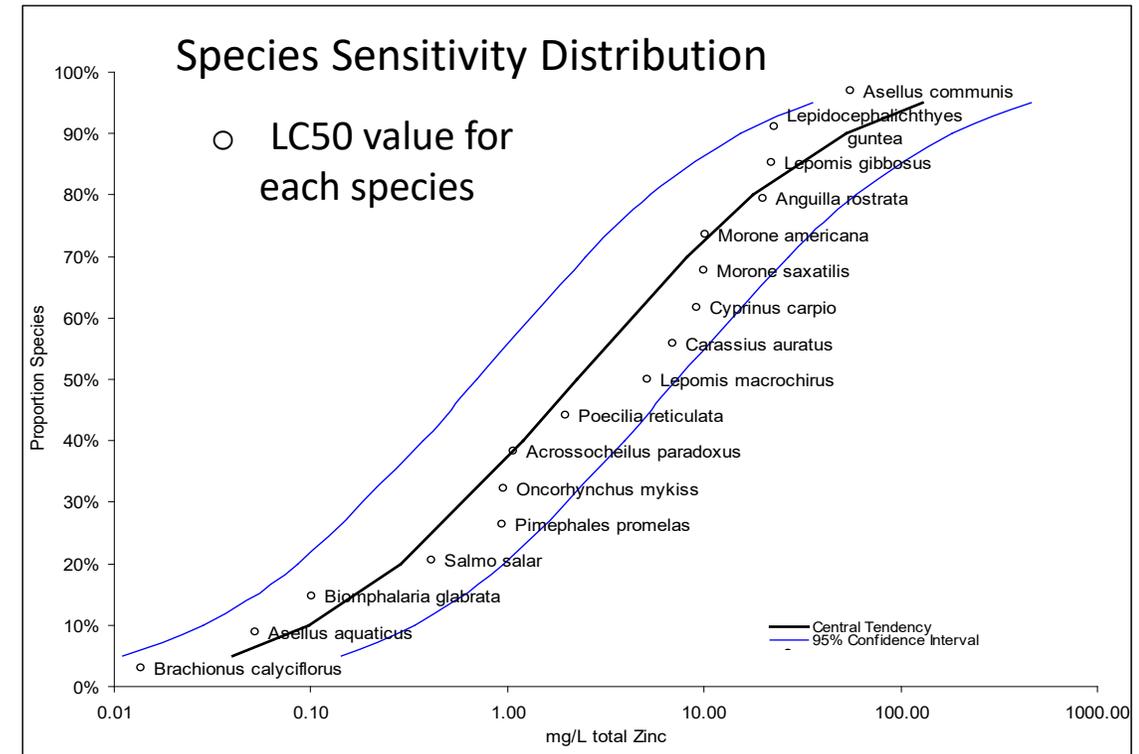
Details	
Mol Wt	191.28
Selected LogKow	2.26
Selected Water Solubility (mg/L)	1910.97
Selected Melting Point (°C)	-45
Estimated LogKow	2.26
Estimated Water Solubility (mg/L)	1910.97
Measured LogKow	2.18
Measured Water Solubility (mg/L)	1911.0
Measured Melting Point (°C)	-45

# Hazard: Individual Species



# Hazard: Multiple Species

Increasing proportion of species affected (LC<sub>50</sub>)



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

Status: Ready

Results:

Fit Distribution

Distribution: normal

Fitting method: maximum likelihood

Goodness of Fit: Iterations: 1000

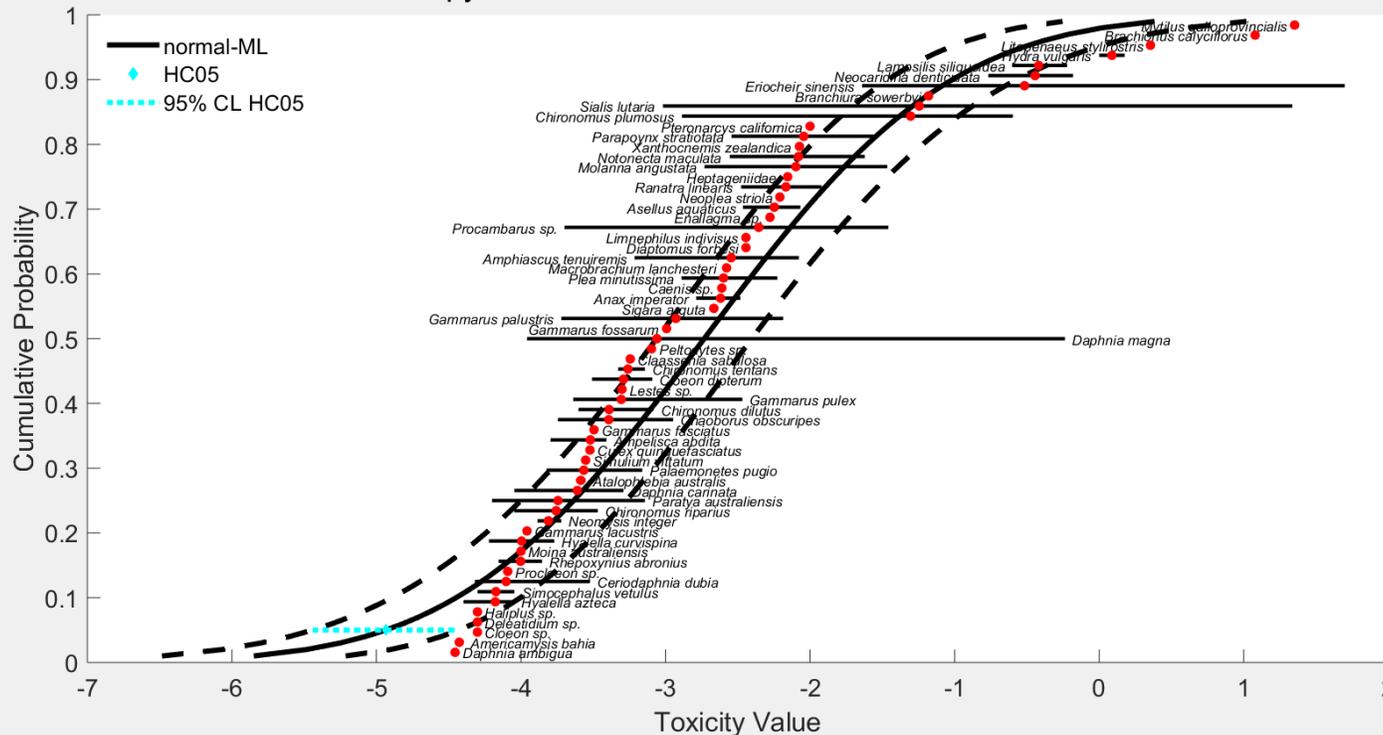
Scaling parameters

Scale to Body Weight

Scaling factor: 1.15

Target weight: 100 g

Chlorpyrifos Inverts MortLC50 ImmbEC50 - SSD = Y



David A. Ettersson  
 Environmental Protection Agency  
 Office of Research and Development  
 National Center for Environmental Toxicology and Exposure  
 Health and Environmental Sciences Division  
 Minneapolis, MN



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# 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/httk/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/>