

Environmental Impact Assessment for Biofuel Associated Chemicals

Chem 234

Chris Vulpe

Spring 2013

Environmental Impact Assessment

- Environmental Fate and Transport (EFT)
- Persistence (P)
- Bioaccumulation (B)
- Toxicity (T)



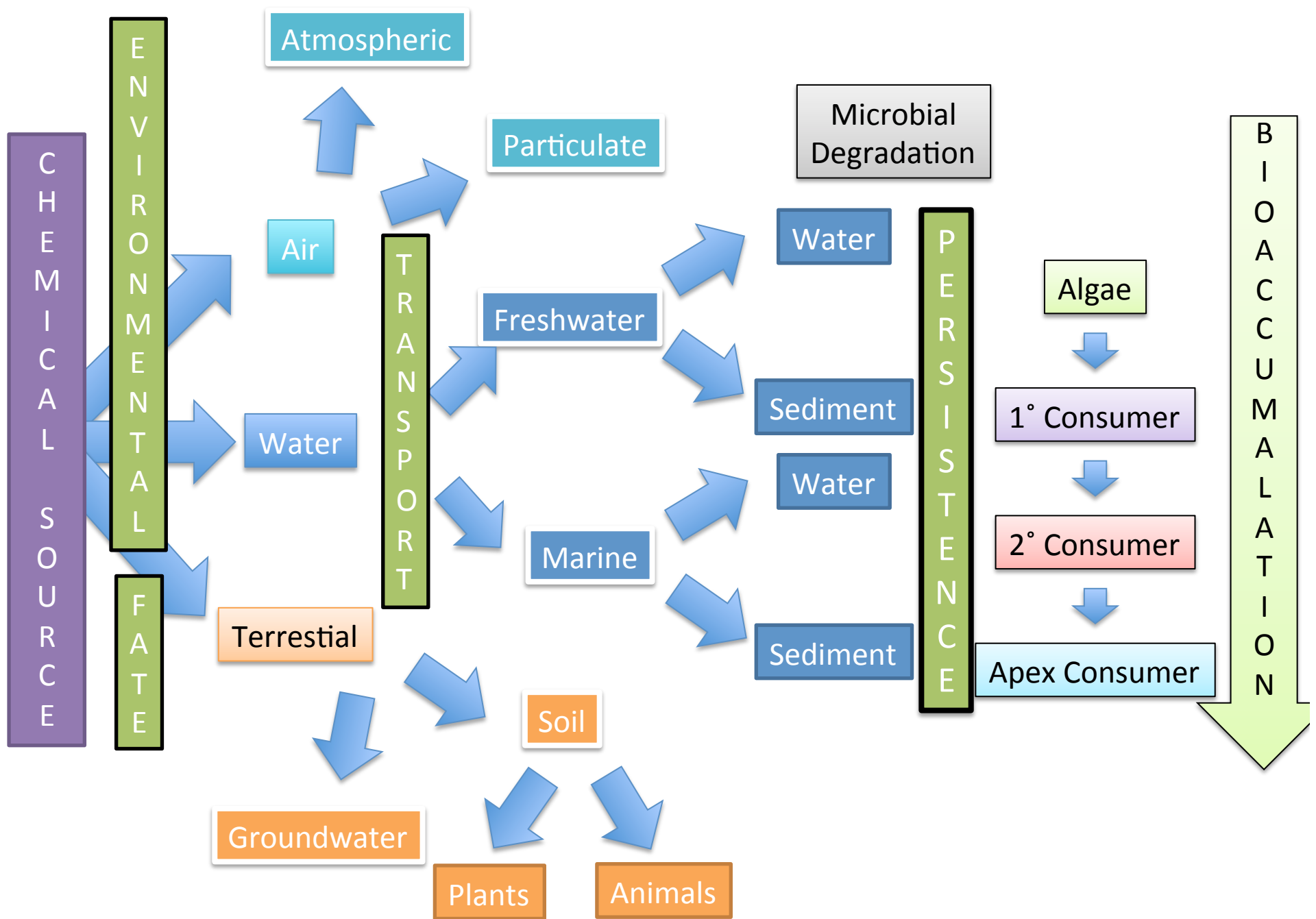
Additional Selected Impacts

Water specific - Eutrophication potential

Air specific - Ambient ozone formation

Particulate formation

Compound	Environmental Fate and Transport	Persistence	Bio-accumulation	Toxicity (acute)	Toxicity (chronic)



Environmental Fate and Transport (EFT)

- Rarely measured
- Use Environmental Fate models to estimate distribution to different media (air, soil, water)
- Use Transport models to estimate movement through each media
- Important for determination of appropriate endpoints (bad things we should worry about) for each chemical.

Environmental Fate and Transport Data

- Environmental Fate Data Base –
 - <http://esc.syrres.com/fatepointer/search.asp>
- eChem Portal property search
 - <http://www.echemportal.org/>

WHAT WE DO / >

[+ Defense](#)

[+ Environment](#)

[+ Intelligence](#)

Products & Services A - Z

SRCTec – Manufacturing/
Lifecycle Support

FatePointers Search Module

> Search

Search below by CAS RN#, substance name, SMILES, or chemical structure with ChemS3. Data sources may be omitted from the search with the buttons to the right.

Enter CAS RN#

or Substance Name
(use * as wildcard)

or SMILES Notation
(use * as wildcard)

Submit Query

> Sources

(Overview of available sources)

+ Physprop	+ Arizona Aquasol
+ ClogP BioByte	+ USDA PestProp
+ ChemFate	+ HPVIS
+ DataLog	+ CHRIP (METI)
+ BioLog	+ OPP Inerts
+ Biodeg	+ OPP Fate
+ HSDB	+ OPP RED
+ HSDB Fate Data	+ U Minn BBD
+ Biodeg Summary	+ NIST
+ OECD SIDS	
Clear all	Check all

> Substructure search using ChemS3

Exact Search

Run Structure Query

Reload last molecule

[Defense](#) > [Environment](#) > [Intelligence](#)[About SRC](#)[What We Do](#)[Careers](#)[Locations](#)[News & Events](#)[Contact Us](#)

WHAT WE DO /

[Chem-Bio](#)[Chemical Fate & Transport](#)[Communications](#)[Counter IED](#)[Cyber Solutions](#)[Electronic Warfare](#)[Free Demos & Databases](#)[Information Assurance](#)[Information Operations](#)[Intelligence / Surveillance /
Reconnaissance](#)[Manufacturing / Lifecycle
Support](#)[Radar & Sensor](#)[Toxicology & Health Risk
Assessment](#)[Training](#)[Products & Services A-Z](#)

Environmental Fate Data Base (EFDB)

Substructure search all of EFDB, TSCATS and PHYSPROP using [ChemS³](#).

Click on one of the buttons below to search the database online.

[Click here for more information.](#)

▶ [DATALOG](#) is a bibliographic file containing 18 types of environmental fate data.

▶ [BIOLOG](#), or the Microbial Degradation/Toxicity File, provides sources of microbial toxicity and biodegradation data.

▶ [CHEMFATE](#) is a data value file containing 25 categories of environmental fate and physical/chemical property information on commercially important chemical compounds. CHEMFATE has not been updated since the mid 1980's. For up-to-date physical properties, please go to the [PHYSPROP database](#).

▶ [BIODEG](#) contains experimental values relating to biodegradation subjects. Records in BIODEG and BIODEG SUMMARY have been updated at varying times from the mid 1980's to approximately 2004 depending upon funding from EPA. The actual time of update can be found by searching individual records in BIODEG or by searching BIODEG SUMMARY by all reliability codes.

▶ [BIODEG SUMMARY](#) provides summary evaluation and reliability codes for different test methods, as well as summaries for biodegradability under aerobic and anaerobic conditions.

Databases last updated on July 16, 2008

EFDB provided on our site through partial support from



PRESS RELEASES /

[SRC Promotes Wendt to
Director of Technology](#)

[LGS Class of 2013 Welcomes
Three SRC Employees](#)

[SRC establishes two new
programs to support stem,
community and increases
support of Honor Flight
program](#)

[Dennis Named One of CNY's
40 Under Forty](#)

[SRC's Thomas Named SRC
and MSS Fellow](#)

• Environmental Fate and Transport Data

eChem Portal property search
<http://www.echemportal.org/>

The screenshot displays the eChemPortal website interface. At the top left is the OECD logo. Below it, a blue banner reads "The Global Portal to Information on Chemical Substances". A left sidebar contains a navigation menu under the "eChemPortal" header, with "Property Search" highlighted. The main content area is titled "Property Search" and includes a "Select Query Block Type" section with a "Load Query" button. Below this is a list of query block types: "Physical and chemical properties", "Environmental fate and pathways", "Ecotoxicological Information", and "Toxicological information". A red arrow points from the "Environmental fate and pathways" option in this list to a detailed view of that category on the right. This detailed view shows a hierarchical list of environmental fate and transport data, including Stability, Biodegradation, Bioaccumulation, and Transport and distribution, with further sub-options for each. At the top right of this detailed view are "Print" and "English" buttons. The footer contains copyright information: "© OECD. All rights reserved. Terms & Conditions | Privacy Policy".

OECD

The Global Portal to Information on Chemical Substances

eChemPortal

- > Home
- > Substance Search
- > Property Search
- > What's new?
- > General Information
- > Participating Databases
- > Roles & Responsibilities
- > Extension of the Portal
- > Linking to eChemPortal
- > Schedules of Assessments
- > Other useful information
- > FAQ
- > Help
- > Contact Us
- > Disclaimer

Property Search

Select Query Block Type

Select a section for which to define query criteria.

Load Query

- + Physical and chemical properties
- + Environmental fate and pathways
- + Ecotoxicological Information
- + Toxicological information

Physical and chemical properties

- Environmental fate and pathways
 - Stability
 - Phototransformation in air
 - Hydrolysis
 - Phototransformation in water
 - Phototransformation in soil
 - Biodegradation
 - Biodegradation in water: screening tests
 - Biodegradation in water and sediment: simulation tests
 - Biodegradation in soil
 - Bioaccumulation
 - Bioaccumulation: aquatic / sediment
 - Bioaccumulation: terrestrial
 - Transport and distribution
 - Adsorption / desorption
 - Henry's Law constant
 - Distribution modelling
 - Environmental data
 - Monitoring data

Print

English

© OECD. All rights reserved. Terms & Conditions | Privacy Policy

EFT Prediction and Models

- EPI suite
 - <http://www.epa.gov/oppt/exposure/pubs/episuitedi.htm>
 - Have to download and run on windows
- **OECD Pov and LRTP Screening Tool**
 - <http://www.oecd.org/env/ehs/risk-assessment/oecdповandlrtpscreeningtool.htm>

Download the Tool and related materials

- [The OECD Pov and LRTP Screening Tool](#) (Version 2.2)

Requirements for the software:

MS Excel 2002 or higher on MS Windows

MS Excel 2004 for Macintosh on Mac OS X (The Tool will not work with MS Excel 2008 for Macintosh.)

- [Manual for the Tool](#)
- [Brochure](#)

A tool for estimating overall persistence (POV) and long-range transport potential (L RTP) of ORGANIC chemicals

The image displays the 'OECD Pov & LRTP Screening Tool' interface, which is overlaid on an Excel spreadsheet. The tool's main menu includes 'Main Menu', 'Help', and 'Preferences'. It is designed for evaluating chemicals based on various parameters.

Select chemicals to evaluate
Simultaneous runs of one database and one chemical are possible.

Databases

Reference Chemicals
Generic PCB Homologues
History

Database Status:

Single Chemical

Name	<input type="text"/>
Molecular mass	<input type="text"/>
Log K_{aw}	<input type="text"/>
Log K_{ow}	<input type="text"/>
Half life in air (h)	<input type="text"/>
Half life in water (h)	<input type="text"/>
Half life in soil (h)	<input type="text"/>

Chemical Status: ☐

☐ Include Monte Carlo Analysis for Single Chemical

Color Codes

	Results already present
	No warnings: calculation possible
	Warnings: calculation still possible
	Errors: calculation impossible
	No data entered

* A manual describing this software is provided on the Help page.

Single Chemical

Chemicals to evaluate database and one chemical are possible.

Name

Molecular mass

Log K_{aw}

Log K_{ow}

Half life in air (h)

Half life in water (h)

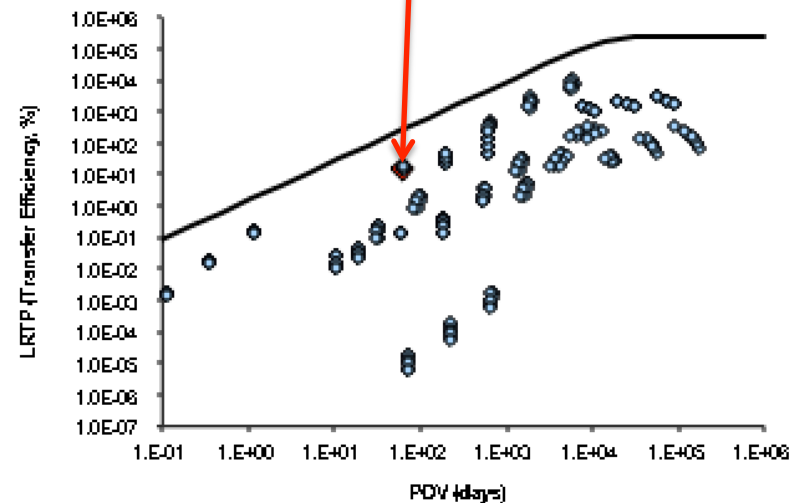
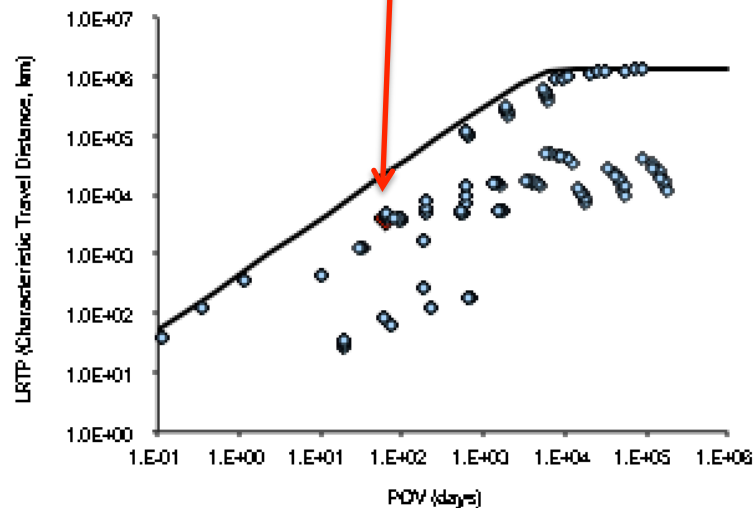
Half life in soil (h)

Chemical Status: ☐

Plots results in comparison to ten compounds with known LRTD and POV (high and low)

Graphical Results

<< Main Menu



Click twice on a point to select it. Do not double-click, but wait between clicks*! Alternatively, use the list below!

Currently highlighted chemical

Name: **a-HCH-1** POV (days): **61.56878**
CTD (km): **3870.393**
TE (%): **14.45401**

Details

Chemical properties

Partition coefficients		Half-lives (hours)	
log K_{ow}	-3.766575649	Air	910.736
log K_{ow}	3.697681703	Water	1024.578
		Soil	1024.578

Select a chemical

From Database: 'Reference Chemicals'

- a-HCH-1**
- a-HCH-10
- a-HCH-11
- a-HCH-12
- a-HCH-13
- a-HCH-14
- a-HCH-15
- a-HCH-16
- a-HCH-17
- a-HCH-18
- a-HCH-19

In Class Exercise

- Pick on chemical of interest to you
- Use the Environmental Fate and LRTP tools to determine or estimate EF and LRTP
- Suggest each team member use different tool
- 15 minutes – report to class on findings/problems

Persistence (P)

- Usually predicted based on physico-chemical properties using computational models
- Degradation and Metabolism databases exist to predict likely metabolites which may have different properties
- Laboratory bio-degradation assays can be used for each media – generally based on use of chemical as carbon source
- Can be measured *in situ* by targeted analytical tools

Persistence/Biodegradation data sources

- eChem Portal property search
 - <http://www.echemportal.org/>
- Environmental Fate Data Base –
 - <http://esc.syrres.com/fatepointer/search.asp>
- University of Minnesota Biocatalysis/
Biodegradation Database
 - <http://umbbd.ethz.ch/>

Persistence/Biodegradation data sources

- eChem Portal property search
 - <http://www.echemportal.org/>

The screenshot displays the eChemPortal website interface. At the top left is the OECD logo. Below it, a blue banner reads "The Global Portal to Information on Chemical Substances". A left sidebar contains a navigation menu with links such as Home, Substance Search, Property Search (highlighted), What's new?, General Information, Participating Databases, Roles & Responsibilities, Extension of the Portal, Linking to eChemPortal, Schedules of Assessments, Other useful information, FAQ, Help, Contact Us, and Disclaimer. The main content area is titled "Property Search" and includes a section "Select Query Block Type" with the instruction "Select a section for which to define query criteria." and a "Load Query" button. Below this are four expandable categories: "Physical and chemical properties", "Environmental fate and pathways", "Ecotoxicological Information", and "Toxicological information". A red arrow points from the "Environmental fate and pathways" category in the main list to a detailed view of this category on the right. This detailed view shows a tree structure of sub-categories: "Physical and chemical properties" (expanded), "Environmental fate and pathways" (collapsed), "Stability" (collapsed), "Biodegradation" (collapsed), "Bioaccumulation" (collapsed), "Transport and distribution" (collapsed), and "Environmental data" (collapsed). Under "Stability", sub-items include "Phototransformation in air", "Hydrolysis", "Phototransformation in water", and "Phototransformation in soil". Under "Biodegradation", sub-items include "Biodegradation in water: screening tests", "Biodegradation in water and sediment: simulation tests", and "Biodegradation in soil". Under "Bioaccumulation", sub-items include "Bioaccumulation: aquatic / sediment" and "Bioaccumulation: terrestrial". Under "Transport and distribution", sub-items include "Adsorption / desorption", "Henry's Law constant", and "Distribution modelling". Under "Environmental data", sub-items include "Monitoring data". A "Print" button and a language dropdown set to "English" are located at the top right of the detailed view.

OECD

The Global Portal to Information on Chemical Substances

eChemPortal

- > Home
- > Substance Search
- > Property Search
- > What's new?
- > General Information
- > Participating Databases
- > Roles & Responsibilities
- > Extension of the Portal
- > Linking to eChemPortal
- > Schedules of Assessments
- > Other useful information
- > FAQ
- > Help
- > Contact Us
- > Disclaimer

Property Search

Select Query Block Type

Select a section for which to define query criteria.

Load Query

- + Physical and chemical properties
- + Environmental fate and pathways
- + Ecotoxicological Information
- + Toxicological information

Physical and chemical properties

- Environmental fate and pathways
 - Stability
 - Phototransformation in air
 - Hydrolysis
 - Phototransformation in water
 - Phototransformation in soil
 - Biodegradation
 - Biodegradation in water: screening tests
 - Biodegradation in water and sediment: simulation tests
 - Biodegradation in soil
 - Bioaccumulation
 - Bioaccumulation: aquatic / sediment
 - Bioaccumulation: terrestrial
 - Transport and distribution
 - Adsorption / desorption
 - Henry's Law constant
 - Distribution modelling
 - Environmental data
 - Monitoring data

Print

English

© OECD. All rights reserved. Terms & Conditions | Privacy Policy

[Defense](#) > [Environment](#) > [Intelligence](#)[About SRC](#)[What We Do](#)[Careers](#)[Locations](#)[News & Events](#)[Contact Us](#)

WHAT WE DO /

[Chem-Bio](#)[Chemical Fate & Transport](#)[Communications](#)[Counter IED](#)[Cyber Solutions](#)[Electronic Warfare](#)[Free Demos & Databases](#)[Information Assurance](#)[Information Operations](#)[Intelligence / Surveillance /
Reconnaissance](#)[Manufacturing / Lifecycle
Support](#)[Radar & Sensor](#)[Toxicology & Health Risk
Assessment](#)[Training](#)[Products & Services A-Z](#)

Environmental Fate Data Base (EFDB)

Substructure search all of EFDB, TSCATS and PHYSPROP using [ChemS³](#).

Click on one of the buttons below to search the database online.

[Click here for more information.](#)

▶ [DATALOG](#) is a bibliographic file containing 18 types of environmental fate data.

▶ [BIOLOG](#), or the Microbial Degradation/Toxicity File, provides sources of microbial toxicity and biodegradation data.

▶ [CHEMFATE](#) is a data value file containing 25 categories of environmental fate and physical/chemical property information on commercially important chemical compounds. CHEMFATE has not been updated since the mid 1980's. For up-to-date physical properties, please go to the [PHYSPROP database](#).

▶ [BIODEG](#) contains experimental values relating to biodegradation subjects. Records in BIODEG and BIODEG SUMMARY have been updated at varying times from the mid 1980's to approximately 2004 depending upon funding from EPA. The actual time of update can be found by searching individual records in BIODEG or by searching BIODEG SUMMARY by all reliability codes.

▶ [BIODEG SUMMARY](#) provides summary evaluation and reliability codes for different test methods, as well as summaries for biodegradability under aerobic and anaerobic conditions.

Databases last updated on July 16, 2008

EFDB provided on our site through partial support from



PRESS RELEASES /

SRC Promotes Wendt to
Director of Technology

LGS Class of 2013 Welcomes
Three SRC Employees

SRC establishes two new
programs to support stem,
community and increases
support of Honor Flight
program

Dennis Named One of CNY's
40 Under Forty

SRC's Thomas Named SRC
and MSS Fellow

Persistence/Bio-degradation prediction tools

- PBT profiler
 - <http://www.pbtprofiler.net/>

Chemicals that Should Not be Profiled [Chemicals with Experimental Data](#)

[Inorganic Chemicals](#) [Reactive Chemicals](#)

[Salts \(Organic Salts\)](#) [High Molecular Weight Compounds](#)

[Chemicals with Unknown or Variable Composition](#)

[Mixtures](#) [Surfactants](#) [Highly Fluorinated Compounds](#)

PBT profiler



[Methodology](#) · [Criteria](#) · [Definitions](#) · [Chemicals That Should Not be Profiled](#)

[Home](#) · [Start a New Profile](#) · [Results](#) · [Terms of Use](#) · [Security](#)



Start a New Profile

Users of the PBT Profiler acknowledge that they have read and accept the [Terms of Use](#)

**To start using the PBT profiler, enter a CAS Registry number or other identifier.
Then, click on the 'Lookup' button to continue.**

Need Help?
[Examples](#)

[Registry numbers and other identifiers](#)
[SMILES Notations](#)
[What the PBT Profiler lookup function does](#)

[Draw your chemical](#)



[Black-and-white version](#)

**NOTE: The estimation modules used by the PBT Profiler have been updated. Some chemicals may produce different profiles than in prior versions.
For a full list of updates see the ["What's new" section](#).**

[Developed by the Environmental Health Analysis Center under contract to the Office of Chemical Safety and Pollution Prevention, U.S. Environmental Protection Agency](#)

Computer Resources Donated by [SRC, Inc.](#)

Ver 2.000 Last Updated September 4, 2012

Bioaccumulation (B)

- Often linked with persistence/biodegradation
 - octanol-water partition coefficient (K_{OW})
 - the ratio of the solubility of a compound in octanol (a non-polar solvent) to its solubility in water (a polar solvent).
 - bioconcentration factor (BCF)
 - ratio of the pollutant concentration in organism to that in water
 - bioaccumulation factor (BAF)
 - the ratio of contaminant concentration measured in biota in the field (or under multiple exposure conditions) to the concentration measured in the surrounding water.
 - biomagnification factor (BMF)
 - ratio of contaminant concentration in biota to that in the surrounding water when the biota was exposed via contaminated food
 - trophic magnification factor (TMF)
 - slope of a regression between the chemical concentration and trophic level of organisms in the food web.

Bioaccumulation Data sources

- ECOTOX
 - <http://cfpub.epa.gov/ecotox/>
- Ambit Database
 - <http://ambit.sourceforge.net/euras/>

Other sources – not too user friendly.

BSAF (Biota-Sediment Accumulation Factor)

http://www.epa.gov/med/Prods_Pubs/bsaf.htm



ECOTOX Database

[Recent Additions](#) | [Contact Us](#)Search: ☐ All EPA ☒ This Area GoYou are here: [EPA Home](#) » ECOTOX

[Home](#)
[About ECOTOX](#)
[Limitations](#)
[Help Center](#)
[Frequent Questions](#)

[Quick Database Query](#)[Advanced Database Query](#)[Data Downloads](#)[Browse Chemicals](#)[Browse Effects](#)[Browse Species](#)[Send Comments](#)

Quick Database Query



Advanced Database Query

Welcome to ECOTOX Release 4.0. The ECOTOX (ECOTOXicology) database provides single chemical toxicity information for aquatic and terrestrial life.

For information on the latest data releases please see the [Recent Additions](#).

View the [Quick User Guide](#) (PDF, 2 p. 244 KB) to help get you started.

You will need to turn off pop-up blockers for this site.

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

NHEERL / Mid-Continent Ecology Division

Other Tools & Databases

- [ASTER](#)
- [BSAF data set](#)
- [Eco-SSL documents](#)
- [Fathead Minnow data set](#)
- [PCB Residue Effects data set](#)
- [Toxicity/Residue](#)



ECOTOX Database

[Recent Additions](#) | [Contact Us](#)Search: ☐ All EPA ☒ This AreaYou are here: [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](#)

Taxonomic Name Entry

[Clear Selections](#)**Search Tip:** [Browse Species Index](#) to find the best input format for
your species information.Kingdom: ☒ Animals ☐ PlantsEnter either species names and/or species num
system allows for both species names and spec
entered in the same query. Place each individua
line. To ensure your final entry is included, end
with a final return (enter key) .

For name searches:

Effect Measurements

[Clear Selections](#)**Search Tip:** Browse the [Effects Index](#) to find the best input format
for your effects.☐ Endpoint Not
Reported (NR)☐ Statistics,
No Endpoint☐ Endpoint Reported☒ Accumulation☐ Cellular☐ Mortality☐ Behavior☐ Ecosystem☐ Physiology☐ Biochemical☐ Growth☐ Population☐ Reproduction

Bioconcentration Factor

**Aquatic Search
Results:**
3096 Records

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 [Next](#)>> [References](#) Page 1 of 43

<u>Spec. Sci. Name</u>	<u>Exp. Type</u>	<u>Media Type</u>	<u>Resp. Site</u>	<u>Endpoint</u>	<u>Trend</u>	<u>Effect</u>	<u>Conc (ug/L)</u>	<u>Stat. Signif.</u>	<u>Ref#</u>	<u>View Details</u>
<u>Spec. Common Name</u>	<u>Chem. Anal.</u>	<u>Loc</u>	<u>Obs. Dur. (Days)</u>	<u>BCF</u>	<u>Eff %</u>	<u>Effect Meas.</u>	<u>Appl. Rate</u>	<u>Sig. Level</u>		

CAS #/Chemical: 50293 - 1,1'-(2,2,2-Trichloroethylidene)bis[4-chlorobenzene]

Algae, Moss, Fungi

Ulva rigida Green Algae	<u>S</u> <u>M</u>	<u>SW</u> <u>LAB</u>	<u>7</u>	<u>BCF</u> <u>152</u>	<u>_____</u>	<u>ACC</u> <u>RSDE</u>	A <u>1000 ug/L</u>	<u>_____</u>	7588	View Details
Ulva rigida Green Algae	<u>S</u> <u>M</u>	<u>SW</u> <u>LAB</u>	<u>7</u>	<u>BCF</u> <u>159</u>	<u>_____</u>	<u>ACC</u> <u>RSDE</u>	A <u>1000 ug/L</u>	<u>_____</u>	7588	View Details
Ulva rigida Green Algae	<u>S</u> <u>M</u>	<u>SW</u> <u>LAB</u>	<u>7</u>	<u>BCF</u> <u>319</u>	<u>_____</u>	<u>ACC</u> <u>RSDE</u>	A <u>1000 ug/L</u>	<u>_____</u>	7588	View Details
Ulva rigida Green Algae	<u>S</u> <u>M</u>	<u>SW</u> <u>LAB</u>	<u>7</u>	<u>BCF</u> <u>1062</u>	<u>_____</u>	<u>ACC</u> <u>RSDE</u>	A <u>1000 ug/L</u>	<u>_____</u>	7588	View Details
Ulva rigida Green Algae	<u>S</u> <u>M</u>	<u>SW</u> <u>LAB</u>	<u>7</u>	<u>BCF</u> <u>1983</u>	<u>_____</u>	<u>ACC</u> <u>RSDE</u>	A <u>1000 ug/L</u>	<u>_____</u>	7588	View Details

Ambit Database

<http://ambit.sourceforge.net/euras/>

ambit

Search [EURAS bioconcentration factor \(BCF\) Gold Standard Database](#)

CAS Registry
number

Enter CAS registry number (hyphenated) or click on the CAS field in the result list

Chemical name

Searches for names that sound like user specified name (e.g. 'naftalen' will hit 'naphthalene')

Reliability score

Enter one of 1,2,3 or MITI or click on the 'Reliability score' field in the result list

Species

Enter species latin name (e.g. *Pimephales promelas*) or click on the species field in the result list

Search

All criteria are combined with 'logical AND'. If no criteria is specified, entire database is retrieved.

substance common name`=naphthalene

[First](#) [Previous](#) Page 1 of 1 [Next](#) [Last](#) Number of results per page 100

#	CAS	Substance common name	Reliability score	Species	Species sex,M/F /MF/nd	Fish weight,g	Fish length,cm	Fish age	Temperature,°C	Job	Tissue analyzed	BCFss ww, Cf/Cw (L/kg)	BCFss lipid,Cf lipid/Cw (L/kg)	BCFk ww,k1/k2	BCFk lipid,BCFk ww/lipid%	Lipid,%
1	91-20-3	naphthalene	1	Cyprinodon variegatus (sheepshead minnow)	MF	2.47	4.7	adult	25	1	whole body	714	7360.824742	999	10307	9.7

Bioaccumulation Prediction

- PBT Profiler - uses the atomic structure to estimate properties of a substance, but focuses on properties relating to persistence, bio-accumulation, and toxicity.
 - <http://www.pbtprofiler.net/>
- ToxPredict – Open tox module
 - <http://www.opentox.org/toxicity-prediction>
 - <http://apps.ideaconsult.net:8080/ToxPredict>
- Vega QSAR
 - <http://www.vega-qsar.eu/use-qsar.html>
 - Need to register and download Java program
 - Need smiles file - get from Chemspider
 - <http://www.chemspider.com/>

Please select the structure(s) for which you would like to apply some OpenTox models.

Draw

Search

Query*

Search mode

- ☒ Auto detect
☐ Exact structure
☐ Substructure search
☐ Similarity search

WELCOME

[Log in](#)

PREDICT

[Search structure](#)

[Upload structure](#)

[View results](#)

BROWSE

[Datasets](#)

[Models](#)

MY WORKSPACE

[My uploads](#)

Predictions

Datasets

[JME Editor courtesy of](#)



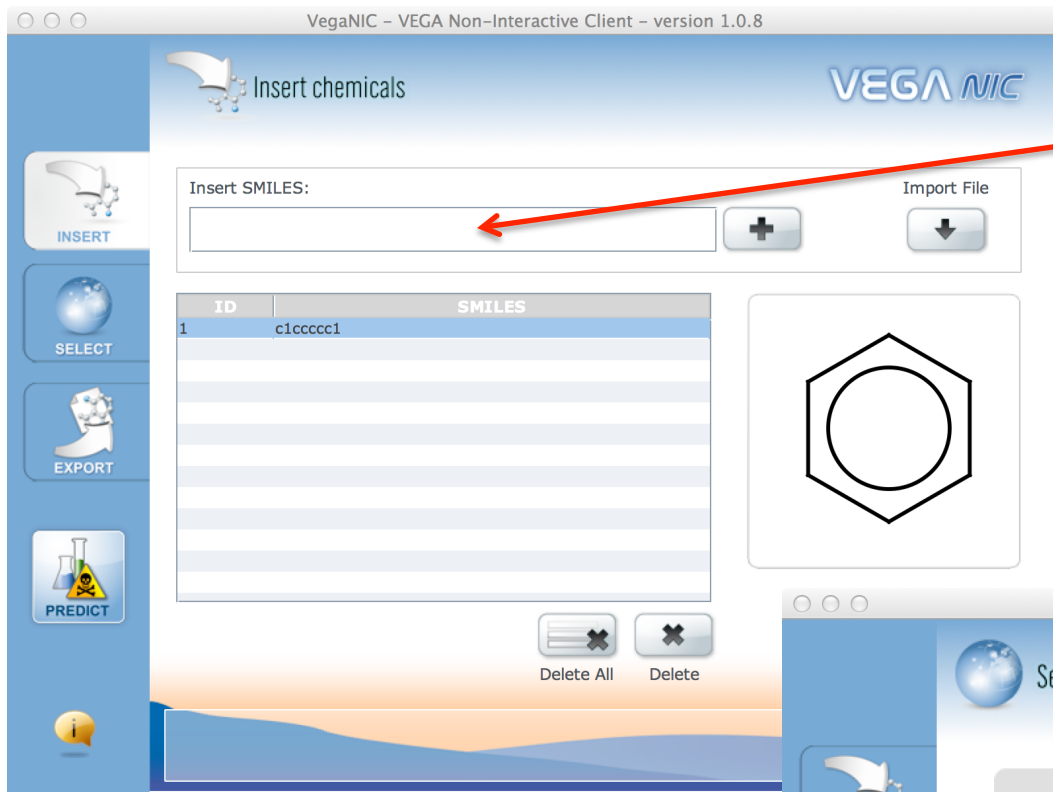
[CADASTER FP7] UI: logKow (TAZ & BTAZ) [Calculate](#)

[CADASTER FP7] logKow_MLRA_[EState], 20560 [Calculate](#)

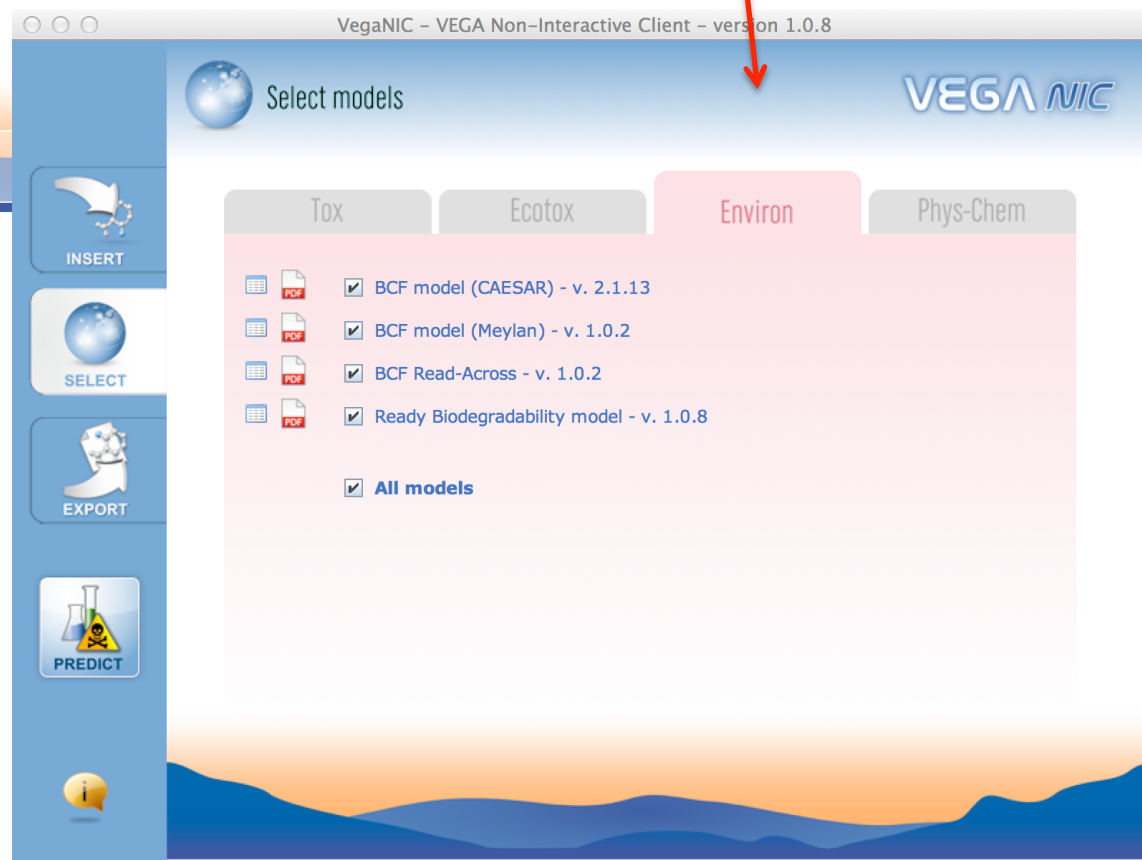
[CADASTER FP7] UI: BCF tutorial [Calculate](#)

[Environmental fate parameters >> Persistence: Biodegradation](#)

START biodegradation and persistence plug-in [Calculate](#)



VEGA





Export results

VEGA *NIC*



INSERT



SELECT



EXPORT



PREDICT



☐ PDF reports (one for each model)

☒ Single PDF report (ordered by model)

/Users/chris/Desktop



☐ Single PDF report (ordered by molecule)

☐ High Resolution

☒ Low Resolution



☐ Plain text files (one for each model)

☐ Summary (single plain text file)

In Class Exercise

- Use same chemical as in previous example
- Use the Persistence and Bioaccumulation tools to determine/estimate persistence and bioaccumulation
- Suggest each team member use different tool
- 15 minutes – report to class on findings/problems

Toxicity (T)

- Most difficult to predict – very rarely measured *in vivo*.
- Empirical data in eco-indicator species used if available
- Important to consider organisms in different trophic levels
- Generally identify the most sensitive species as indicator of potential ecosystem toxicity

Toxicity Data Sources


Authoritative Body Lists and Lists of Lists

- Pharos project
 - <http://www.pharosproject.net>

Toxicity Databases

- EPA ecotox Database
 - <http://cfpub.epa.gov/ecotox>
- Toxnet – 14 databases
 - <http://toxnet.nlm.nih.gov/>
- eChem Portal –OECD 17 databases
 - <http://www.echemportal.org/>
- ESIS : European chemical Substances Information System -aggregates data from a number of other European databases
 - <http://esis.jrc.ec.europa.eu/>

Ecotox Database search



Home

About ECOTOX

Limitations

Help Center

Frequent Questions

Quick Database Query

Advanced Database Query

Data Downloads

Browse Chemicals

Browse Effects

Browse Species


Send Comments

U.S. ENVIRONMENTAL PROTECTION AGENCY


ECOTOX Database

[Recent Additions](#) | [Contact Us](#) **Search:** ☐ All EPA ☒ This Area

You are here: [EPA Home](#) » ECOTOX



Quick Database Query



Advanced Database Query

Welcome to ECOTOX Release 4.0. The ECOTOX (ECOTOXicology) database provides single chemical toxicity information for aquatic and terrestrial life.

For information on the latest data releases please see the [Recent Additions](#).

View the [Quick User Guide](#) (PDF, 2 p. 244 KB) to help get you started.

You will need to turn off pop-up blockers for this site.


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

NHEERL / Mid-Continent Ecology Division

Other Tools & Databases

- [ASTER](#)
- [BSAF data set](#)
- [Eco-SSL documents](#)
- [Fathead Minnow data set](#)
- [PCB Residue Effects data set](#)
- [Toxicity/Residue](#)

Select a
TOXNET
Database
to Search

 United States
National Library
of Medicine

TOXNET

Toxicology Data Network

[TOXNET PDA Access](#) | [SIS Home](#) | [About Us](#) | [Site Map & Search](#) | [Contact Us](#)

[Env. Health & Toxicology](#) | [TOXNET](#)

TOXNET - Databases on toxicology, hazardous chemicals, environmental health, and toxic releases.

Select Database

- [ChemIDplus](#)
- [HSDB](#)
- [TOXLINE](#)
- [CCRIS](#)
- [DART](#)
- [GENETOX](#)
- [IRIS](#)
- [ITER](#)
- [LactMed](#)
- [Multi-Database](#)
- [TRI](#)
- [Haz-Map](#)
- [Household Products](#)
- [TOXMAP](#)

Search All Databases

Enter term(s) to search all databases.


(e.g. asthma air pollution, ibuprofen fever, vinyl chloride)

[Search](#) [Clear](#) [Help](#)

TOXNET Search Options

- Search all databases: Enter term(s) in box above
- Search a specific database: Click database at left
- Database description: Click on the [?](#)

Env. Health & Toxicology



Portal to
environmental
health and
toxicology
resources

[VISIT SITE](#)

Support Pages

- ▶ [Help](#)
- ▶ [TOXNET FAQ](#)
- ▶ [TOXNET Update Status](#)
- ▶ [Fact Sheet](#)
- ▶ [Database Description](#)
- ▶ [Training Manual & Schedule](#)
- ▶ [News](#)

Additional Resource

- [CPDB](#)
- [CTD](#)

Search all
Databases

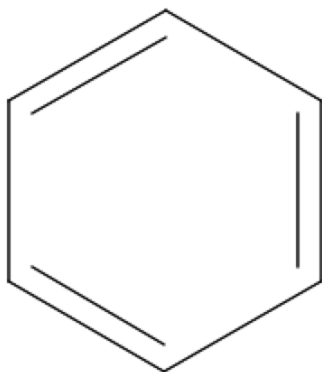
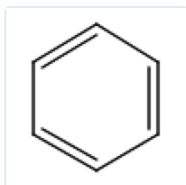
Link to
EH/Tox
Portal

Support
Pages

toxnet.nlm.nih.gov

Eco-Toxicity Prediction

- ECOSAR -Ecological Structure-Activity Relationship estimator, attempts to estimate the toxicity potential of a substance based on its atomic structure
 - <http://www.epa.gov/oppt/newchems/tools/21ecosar.htm>
 - Need to download and run on windows
- AIM, or Analog Identification Methodology –estimates toxicity hazard by comparing an unknown chemical to analogs which have been tested
 - <http://www.epa.gov/oppt/sf/tools/aim.htm>
 - Need to download and run on windows
- PBT Profiler - uses the atomic structure to estimate properties of a substance, but focuses on properties relating to persistence, bio-accumulation, and toxicity.
 - <http://www.pbtprofiler.net/>
- ToxPredict – Open tox module
 - <http://www.opentox.org/toxicity-prediction>
 - <http://apps.ideaconsult.net:8080/ToxPredict>



[Download](#)
[Browse all](#)

CASRN	71-43-2
EINECS	200-753-7
IUPAC name	benzene
Chemical Name	benzene
SMILES	c1ccccc1
Standard InChI	InChI=1S/C6H6/c1-2-4-6-5-3-1/h1-6H
Standard InChI key	UHOVQNZJYSORNB-UHFFFAOYSA-N
REACH registration date	30.11.2010

Predictions Datasets

Run All

EPAFM LC50 fish OpenTox model created with SCR regression model [Calculate](#)

[CADASTER FP7] Algae_UIDRAGON_SPLIT [Calculate](#)

[CADASTER FP7] HMGU: EC50 Daphnia (TAZ & BTAZ) [Calculate](#)

[CADASTER FP7] HMGU: EC50 Algae (TAZ & BTAZ) [Calculate](#)

[CADASTER FP7] HMGU: LC50 Fish (TAZ & BTAZ) [Calculate](#)

[CADASTER FP7] HMGU: Abiotic degradation in water [Calculate](#)

[CADASTER FP7] HMGU: Atmospheric OH Rate [Calculate](#)

[CADASTER FP7] HMGU: Koc [Calculate](#)

[CADASTER FP7] HMGU: Photolysis rate [Calculate](#)

[CADASTER FP7] Aquatic tox (fish) [Calculate](#)

[CADASTER FP7] Aquatic tox (daphnia) [Calculate](#)

[CADASTER FP7] Aquatic tox (2nd fish) [Calculate](#)

IST DSSTox Carcinogenic Potency DBS SingleCellCall [Calculate](#)

IST EPA v4b Fathead Minnow Acute Toxicity (LC50_mmol) [Calculate](#)

WELCOME

Log in

PREDICT

Search stru

Upload stru

View resul

BROWSE

Datasets

Models

MY WORKSP

My uploads

In Class Exercise

- Use same chemical as in previous example
- Use the toxicity tools to determine/estimate toxicity of chemical
- Suggest each team member use different tool
- 15 minutes – report to class on findings/problems

Finish Hazard Trait tables

- Use the tools outlined for EFT and PBT to complete the Hazard Trait tables for your chemicals of interest