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)

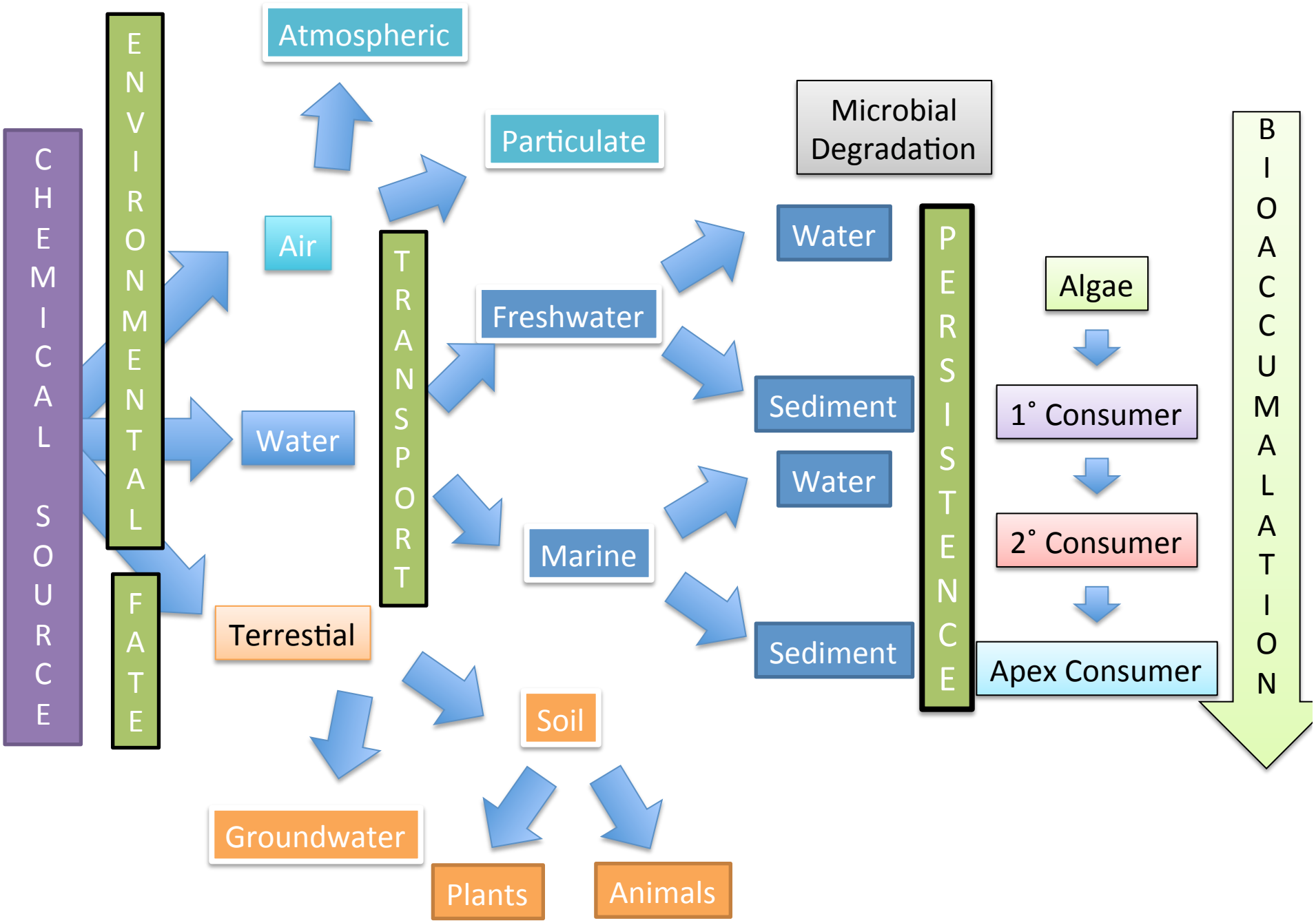
Additional Selected Impacts

Water specific -Eutrophication potential

Air specific - Ambient ozone formation

Particulate formation

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


CHEMICAL SOURCE
ENVIRONMENTAL FATE
Atmospheric
Particulate
Air
Water
Terrestial
TRANSPORT
Freshwater
Marine
Groundwater
Soil
Plants
Animals
Water
Sediment
Water
Sediment
Microbial Degradation
PERSISTENCE
Algae
1° Consumer
2° Consumer
Apex Consumer
BIOACCUMALATION

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

Clear all | Check all

Substructure search using ChemS3

Exact Search

Run Structure Query

Reload last molecule

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 ChemS^3.

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

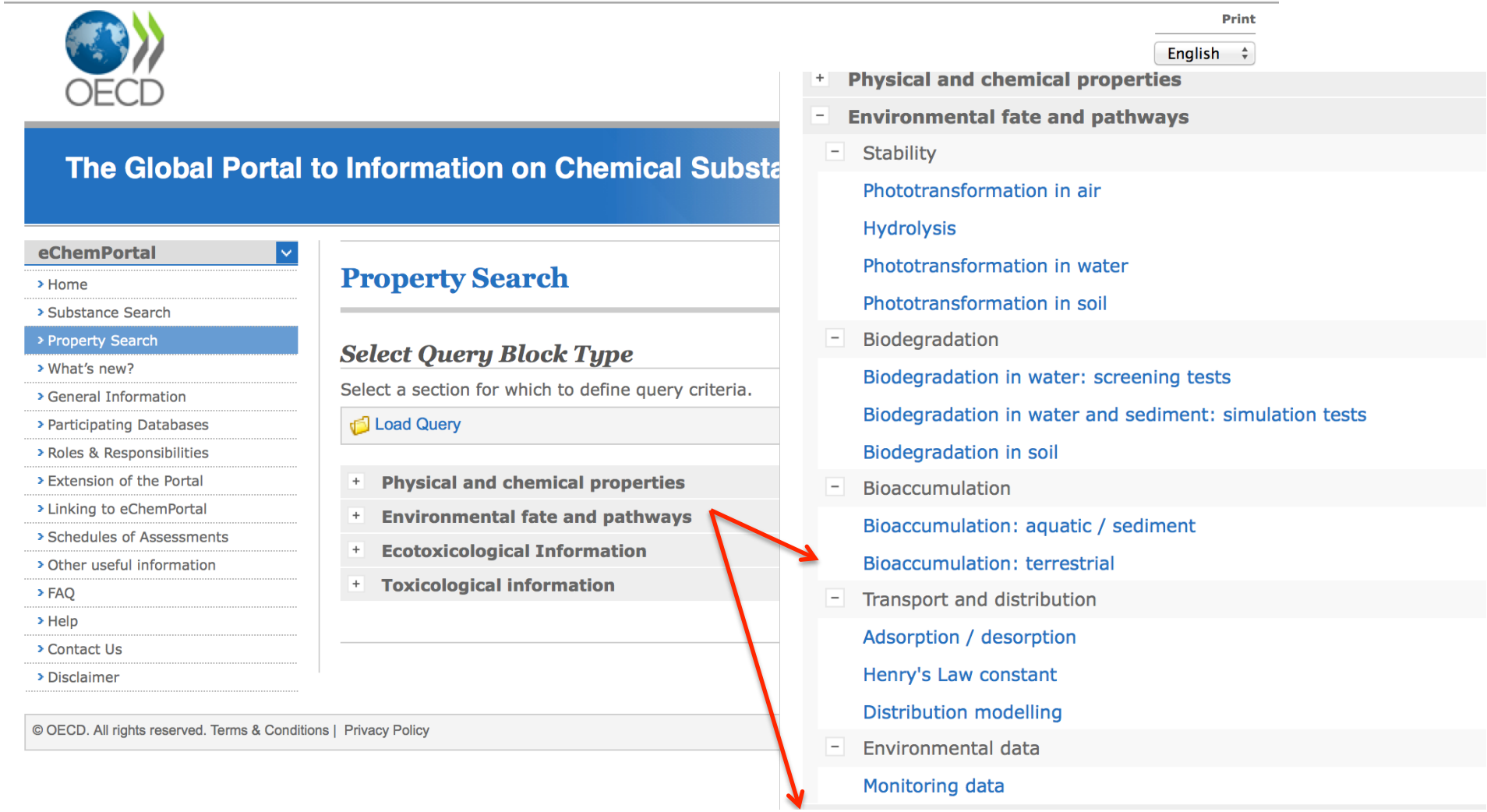
EFDB provided on our site through partial support from EPA, Procter&Gamble, and DUPONT

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

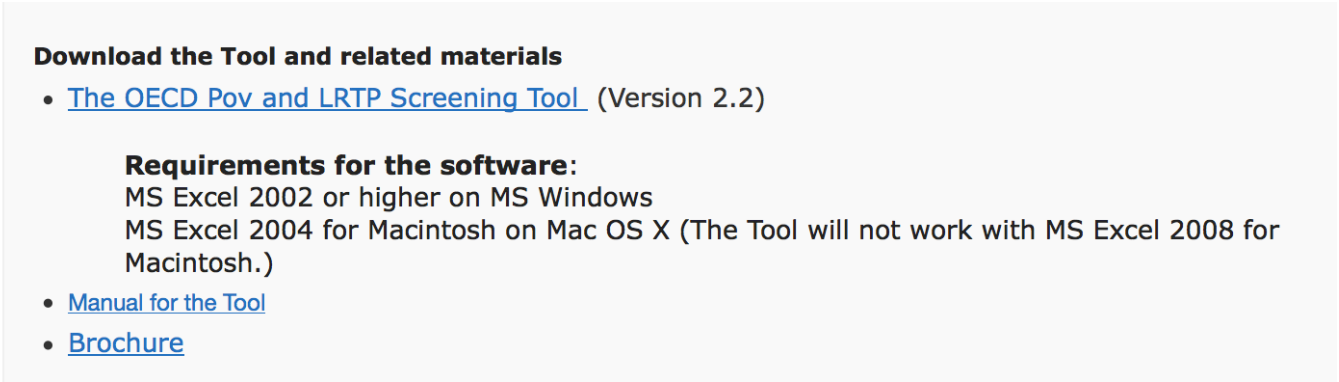
- Environmental Fate and Transport Data

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



EFT Prediction and Models

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

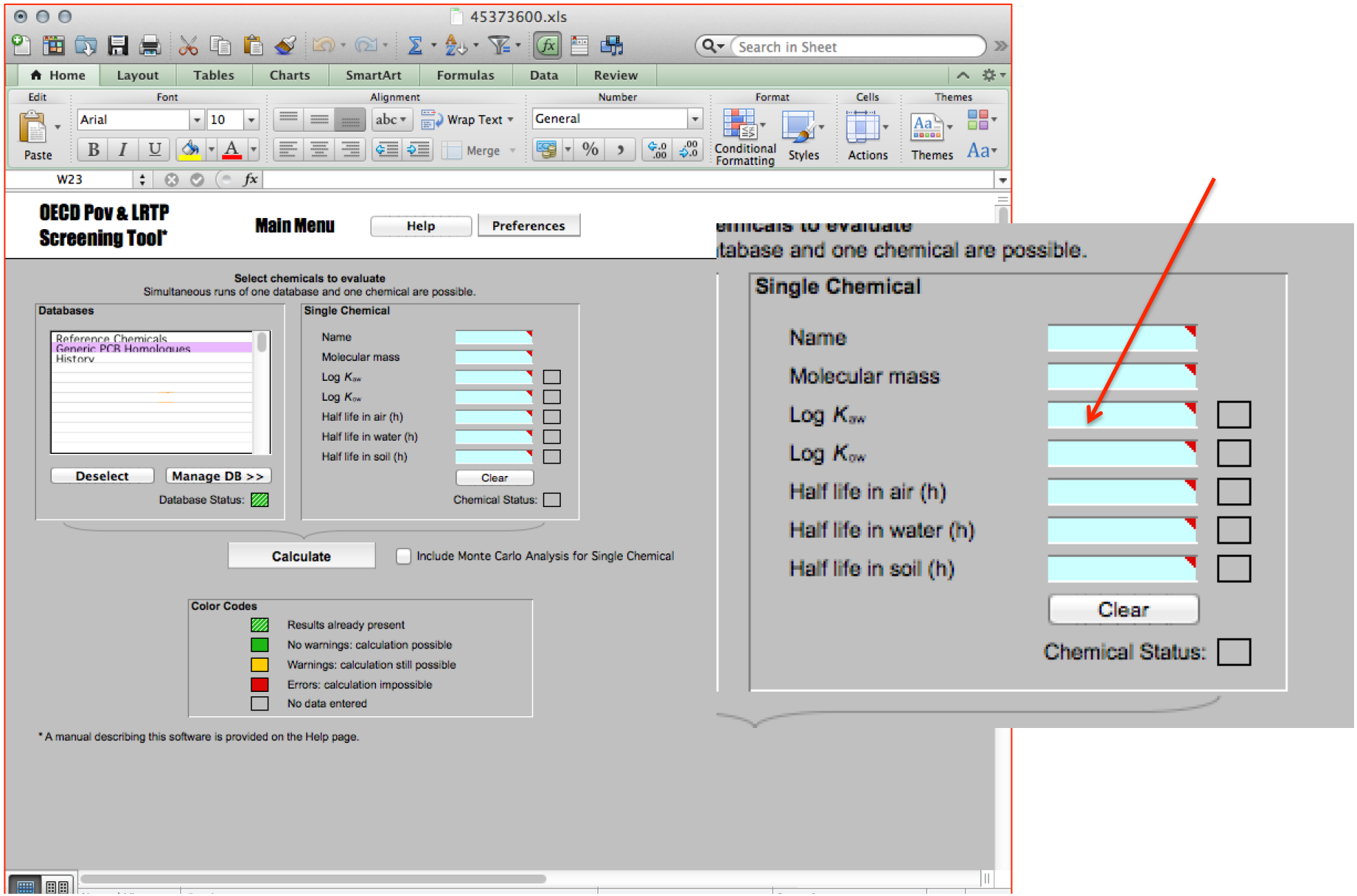


Download the Tool and related materials

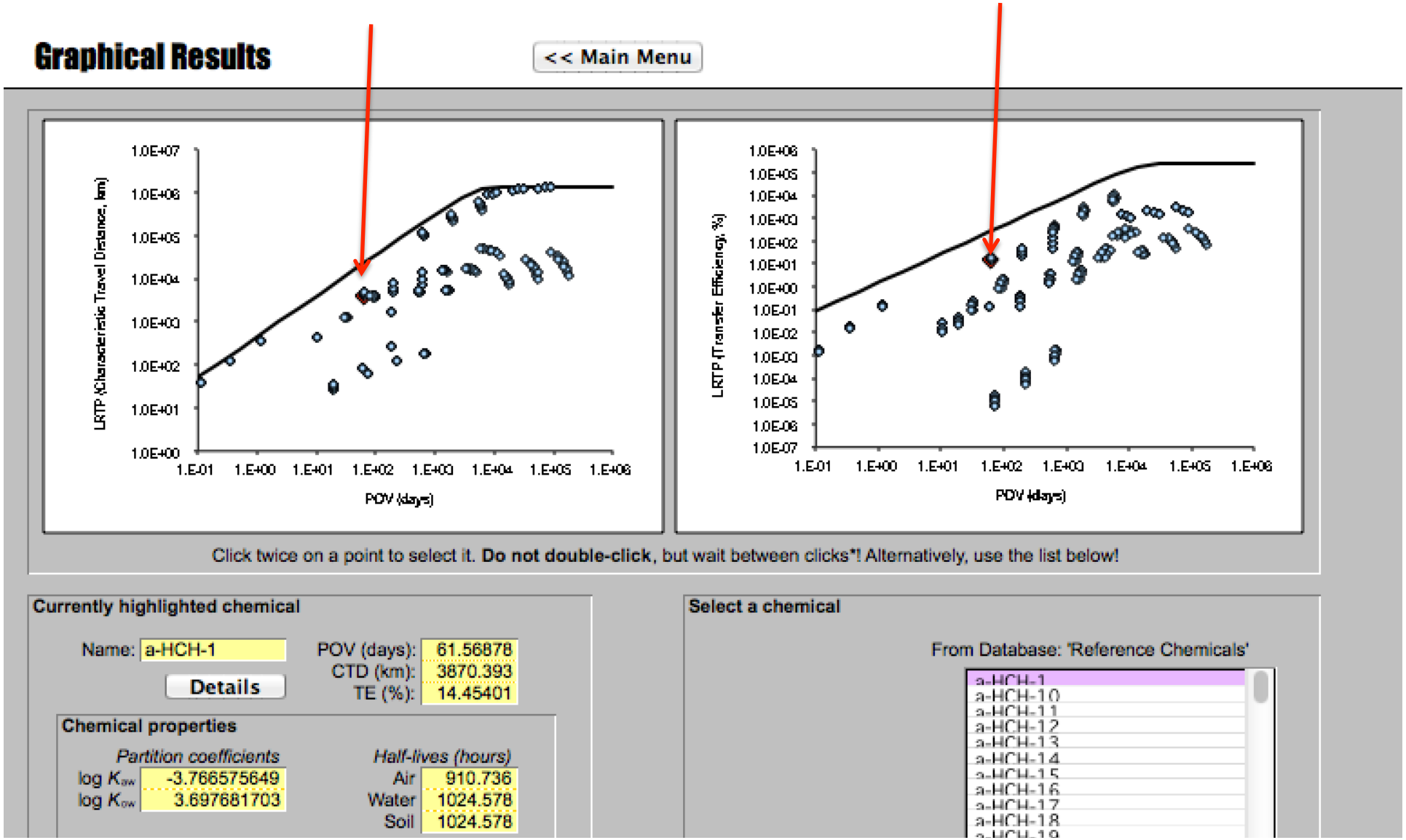
- The OECD Pov and LRTP Screening Tool (Version 2.2)

  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 (**P**OV) and long-range transport potential (LRTP) of ORGANIC chemicals



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



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/

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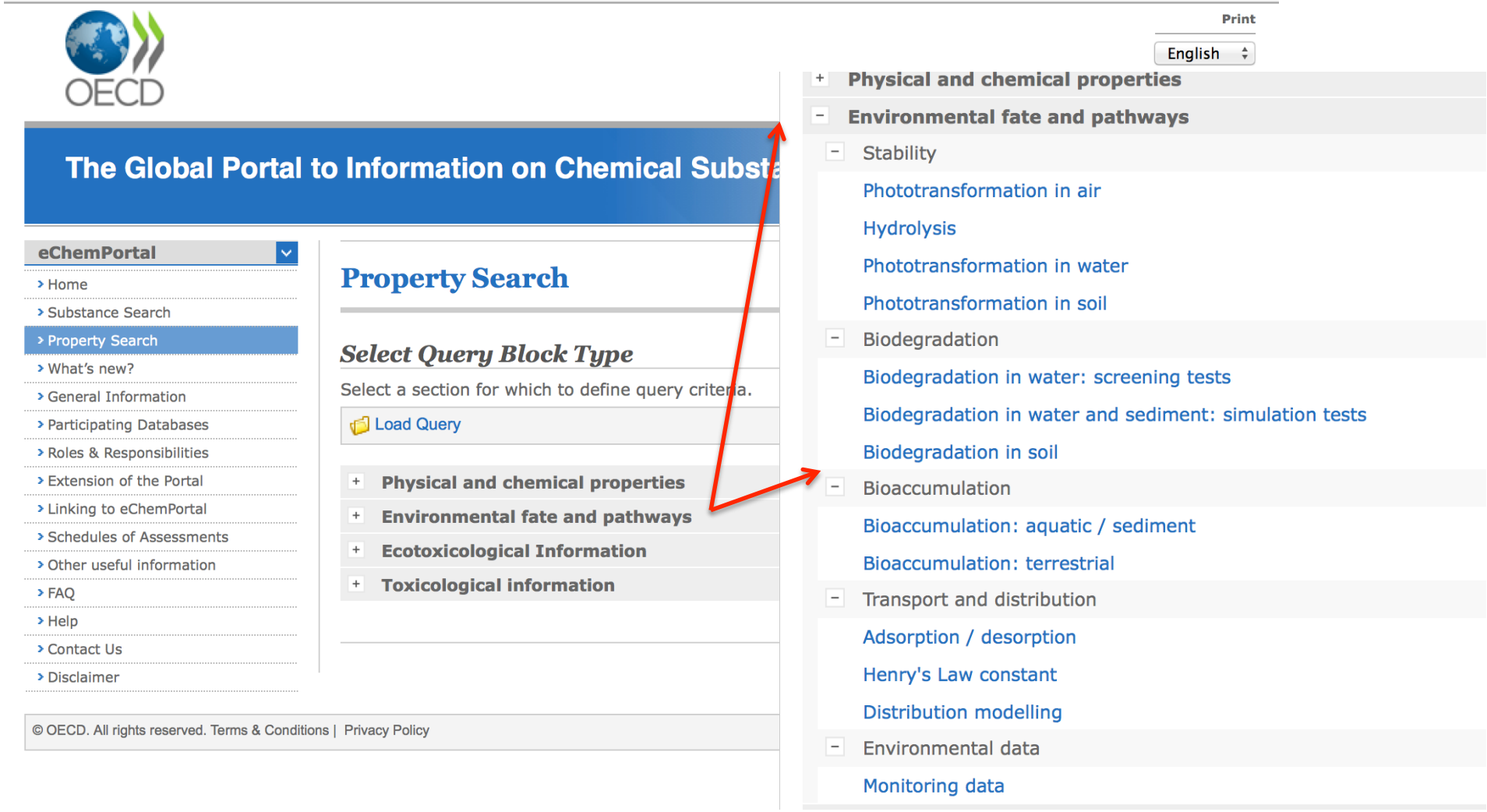

WHAT WE DO /

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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

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

benzene Lookup

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 then 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

U.S. ENVIRONMENTAL PROTECTION AGENCY

ECOTOX Database

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Recent Additions | Contact Us **Search:** All EPA This Area Go

You 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

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.

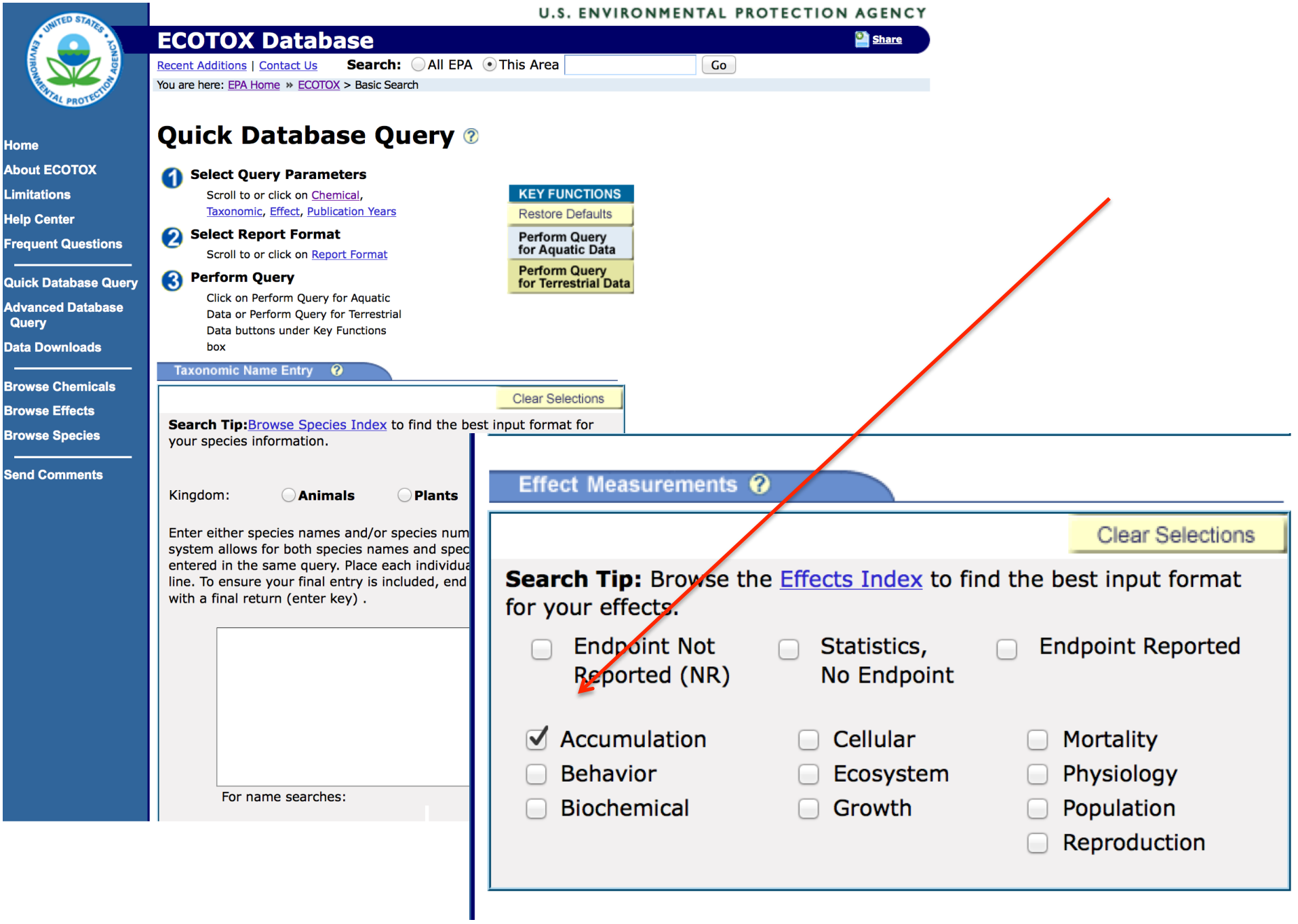
You will need to turn off pop-up blockers for this site.

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


U.S. ENVIRONMENTAL PROTECTION AGENCY
ECOTOX Database
Share
Recent Additions | Contact Us
Search: All EPA This Area
Go
You are here: EPA Home » ECOTOX > Basic 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
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 Plants
Enter 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
Behavior
Biochemical
Cellular
Ecosystem
Growth
Mortality
Physiology
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

Spec. Sci. Name / Spec. Common Name	Exp. Type / Chem. Anal.	Media Type / Loc	Resp. Site / Obs. Dur. (Days)	Endpoint / BCF	Trend / Eff %	Effect / Effect Meas.	Conc (ug/L) / Appl. Rate	Stat. Signif. / Sig. Level	Ref#	View Details
CAS #/Chemical: 50293 - 1,1'-(2,2,2-Trichloroethylidene)bis[4-chlorobenzene]										
Algae, Moss, Fungi										
Ulva rigida Green Algae	S M	SW LAB	7	BCF 152		ACC RSDE	A 1000 ug/L		7588	View Details
Ulva rigida Green Algae	S M	SW LAB	7	BCF 159		ACC RSDE	A 1000 ug/L		7588	View Details
Ulva rigida Green Algae	S M	SW LAB	7	BCF 319		ACC RSDE	A 1000 ug/L		7588	View Details
Ulva rigida Green Algae	S M	SW LAB	7	BCF 1062		ACC RSDE	A 1000 ug/L		7588	View Details
Ulva rigida Green Algae	S M	SW LAB	7	BCF 1983		ACC RSDE	A 1000 ug/L		7588	View Details

Ambit Database

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

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`=**napthalene**

First Previous **Page** 1 of 1 Next Last Number of results per page 100

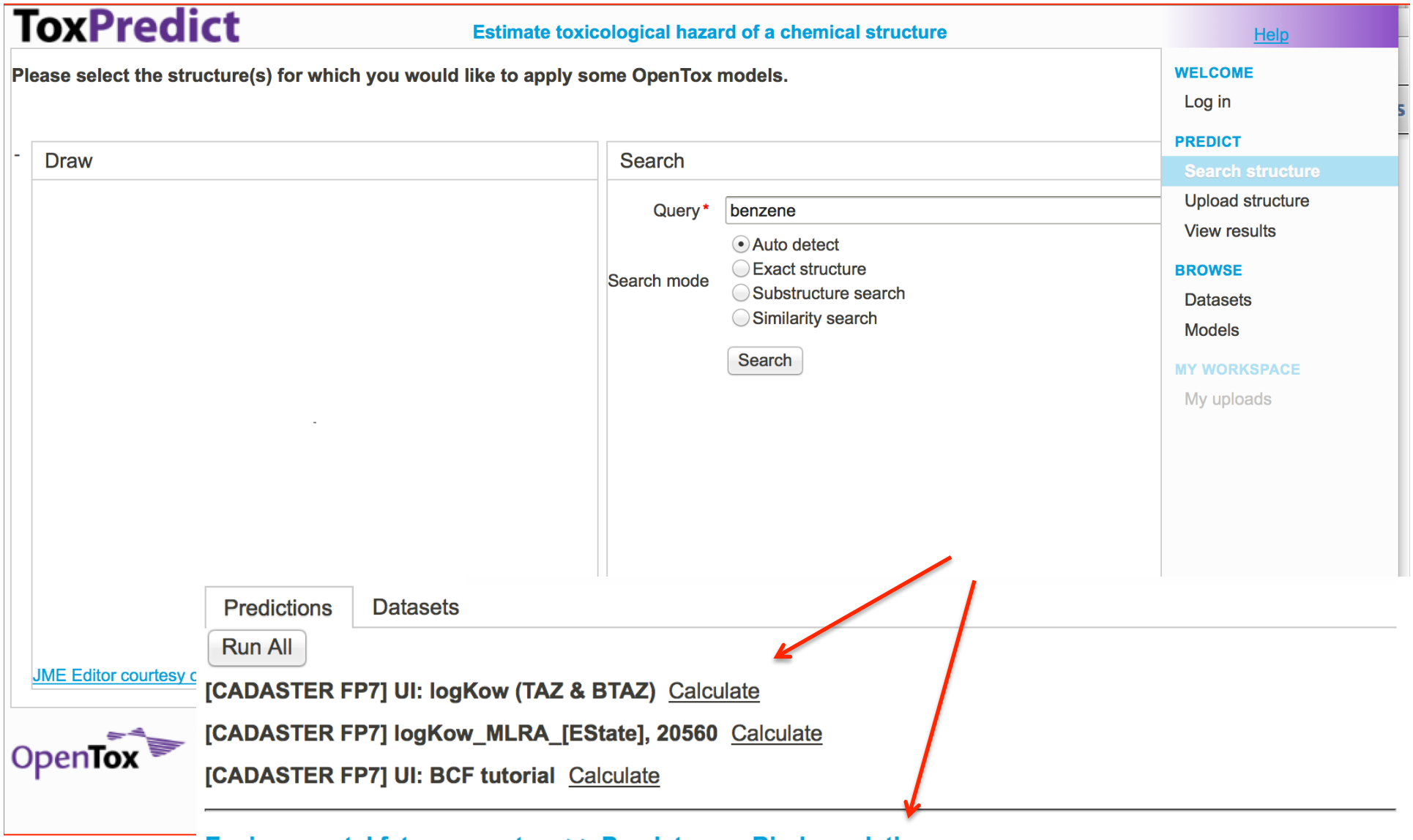
#	CAS	Substance common name	Reliability score	Species	Species sex,M/F/MF/nd	Fish weight,g	Fish length,cm	Fish age	Temperature,°C	ob	Tissue analyzed	BCFss ww Cf/Cw (L/kg)	BCFss lipid,Cf lipid/Cw (L/kg)	BCFk ww,k1/k2	BCFk lipid,BCFk ww/lipid%	Lipid,%
1	91-20-3	naphthalene	1	*Cyprinodon variegatus (sheepshead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

Bioaccumulation Prediction

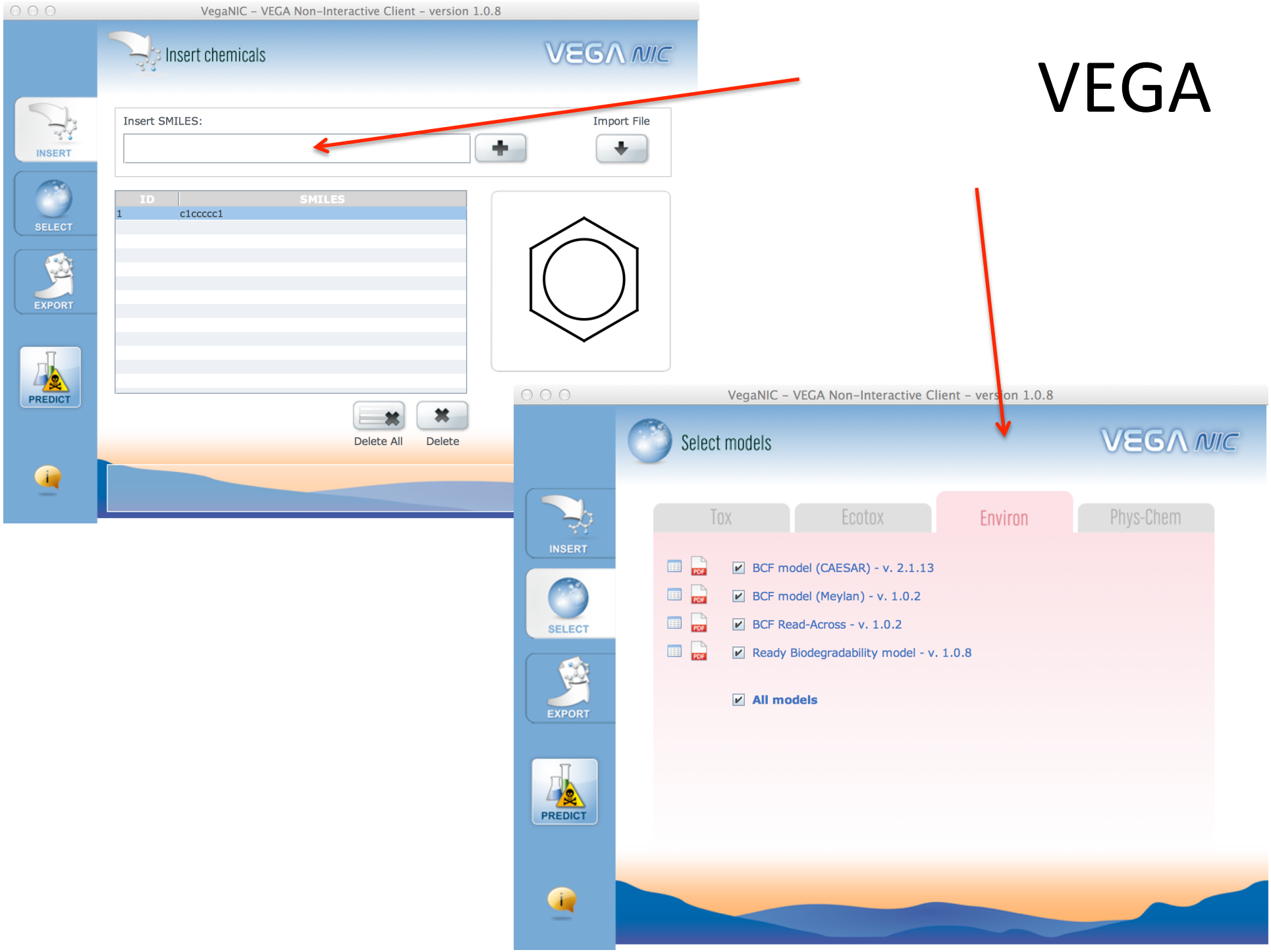
- PBT Profiler - uses the atomic structure to estimate properties of a substance,but focuses on properties relating to persistence, bio-accumulation, and toxicity.
  - http://www.pbtprofiler.net/

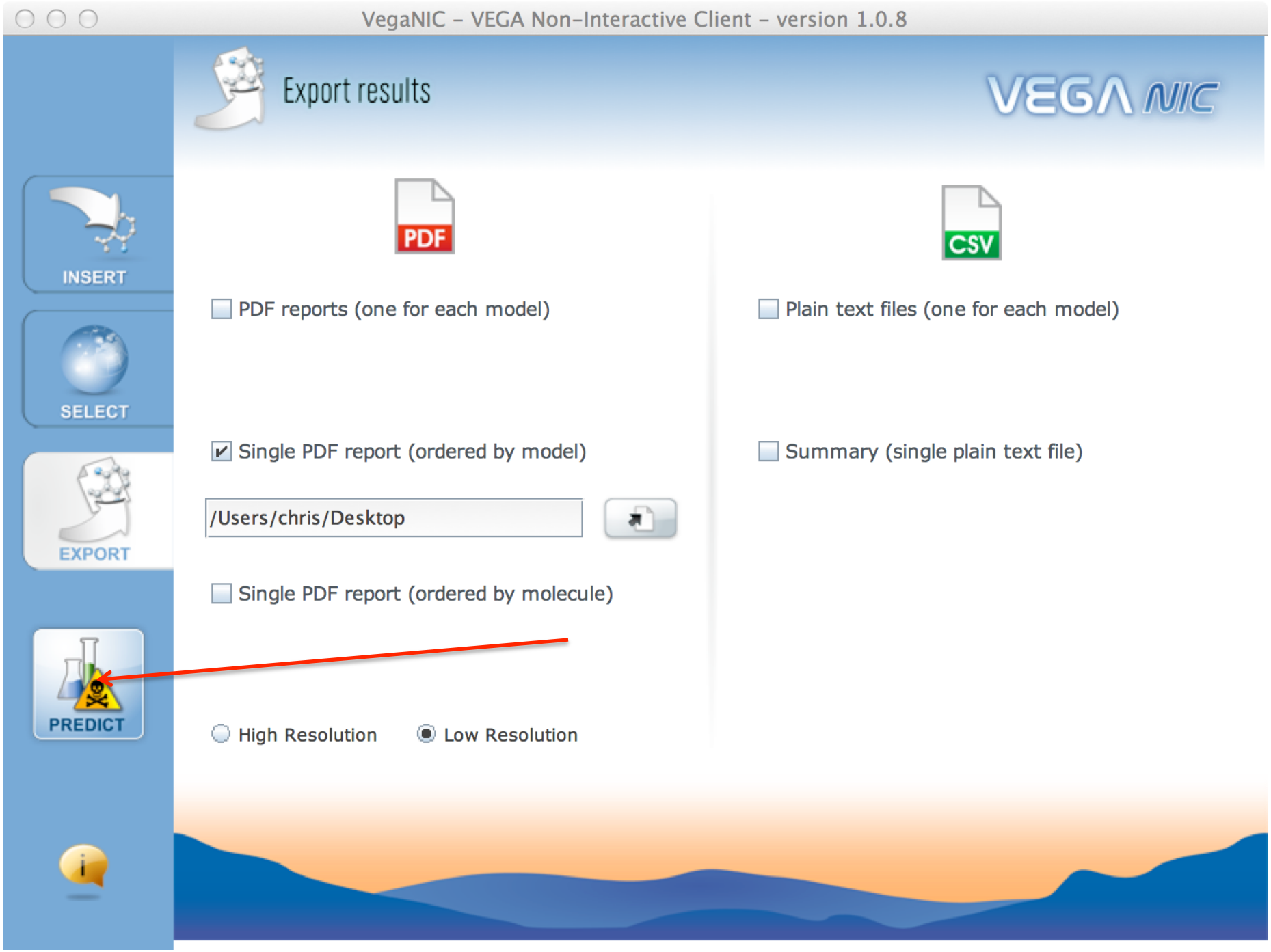
- ToxPredict – Open tox module
  - http://www.opentox.org/toxicity-prediction
  - http://apps.ideaconsult.net:8080/ToxPredict

- 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/


ToxPredict
Estimate toxicological hazard of a chemical structure
Help
Please select the structure(s) for which you would like to apply some OpenTox models.
Draw
Search
Query *
benzene
Search mode
Auto detect
Exact structure
Substructure search
Similarity search
Search
WELCOME
Log in
PREDICT
Search structure
Upload structure
View results
BROWSE
Datasets
Models
MY WORKSPACE
My uploads
JME Editor courtesy
OpenTox
Predictions
Datasets
Run All
[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


VegaNIC – VEGA Non-Interactive Client – version 1.0.8
Insert chemicals
VEGA NIC
INSERT
SELECT
EXPORT
PREDICT
Insert SMILES:
Import File
ID
SMILES
1
c1ccccc1
Delete All
Delete
VegaNIC – VEGA Non-Interactive Client – version 1.0.8
Select models
VEGA NIC
INSERT
SELECT
EXPORT
PREDICT
Tox
Ecotox
Environ
Phys-Chem
BCF model (CAESAR) - v. 2.1.13
BCF model (Meylan) - v. 1.0.2
BCF Read-Across - v. 1.0.2
Ready Biodegradability model - v. 1.0.8
All models


VegaNIC - VEGA Non-Interactive Client - version 1.0.8
Export results
VEGA NIC
INSERT
SELECT
EXPORT
PREDICT
PDF
CSV
PDF reports (one for each model)
Plain text files (one for each model)
Single PDF report (ordered by model)
Summary (single plain text file)
/Users/chris/Desktop
Single PDF report (ordered by molecule)
High Resolution
Low Resolution

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

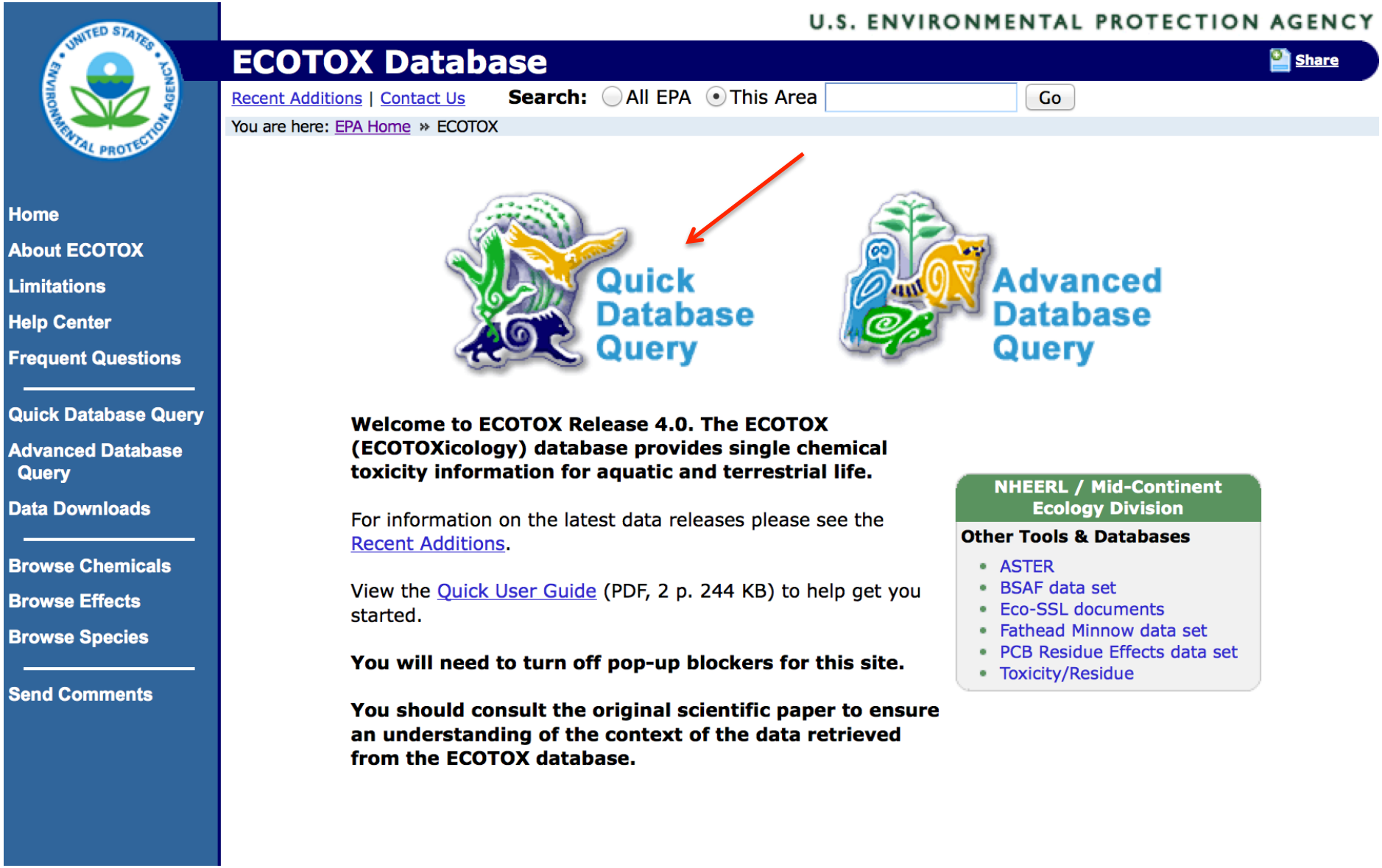
- EPA ecotox Database
  - http://cfpub.epa.gov/ecotox

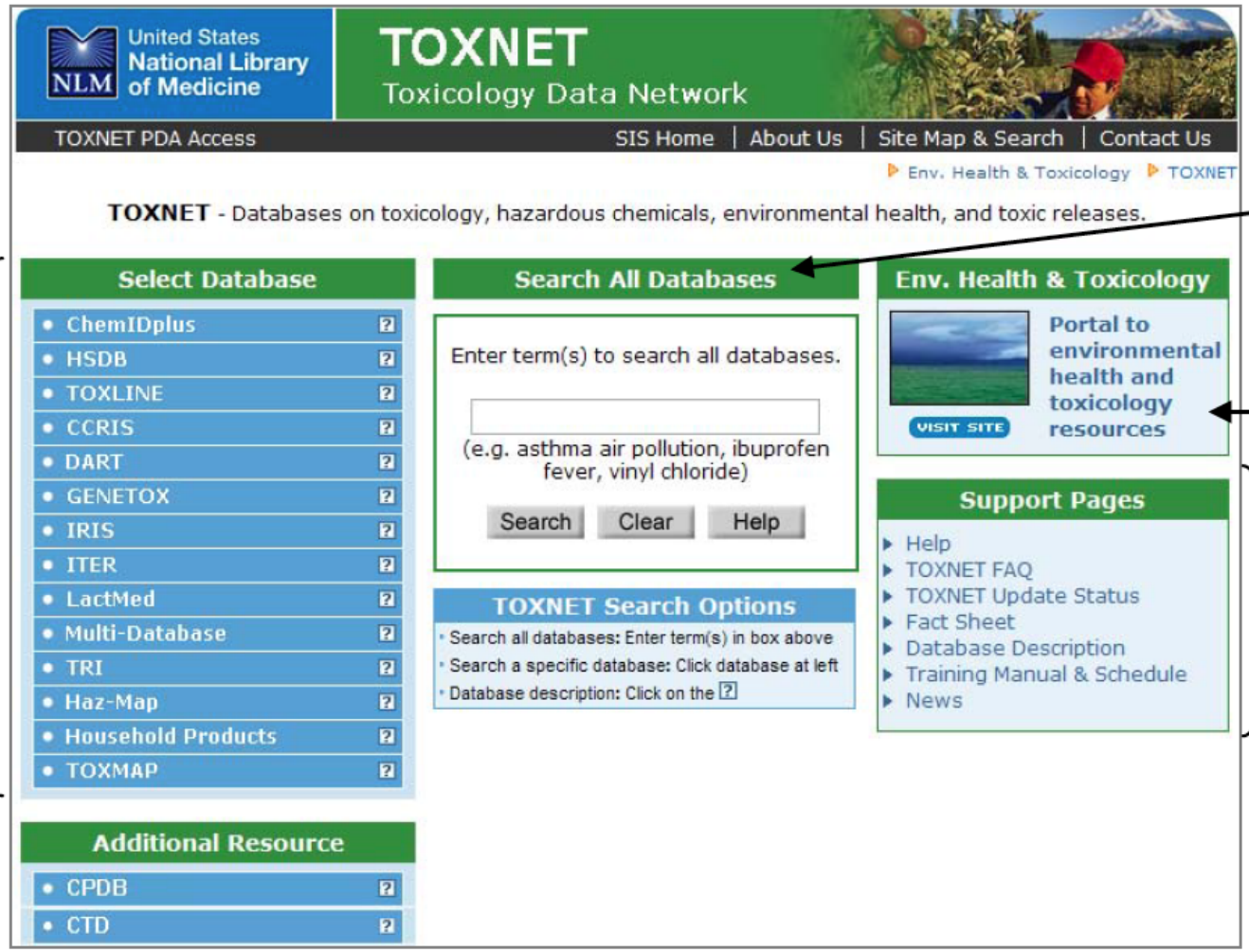
- Toxnet – 14 databases
  - http://toxnet.nlm.nih.gov/

- 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





Search all Databases

Link to EH/Tox Portal

Support Pages

Select a TOXNET Database to Search

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.
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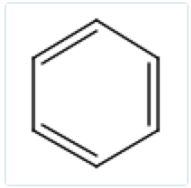
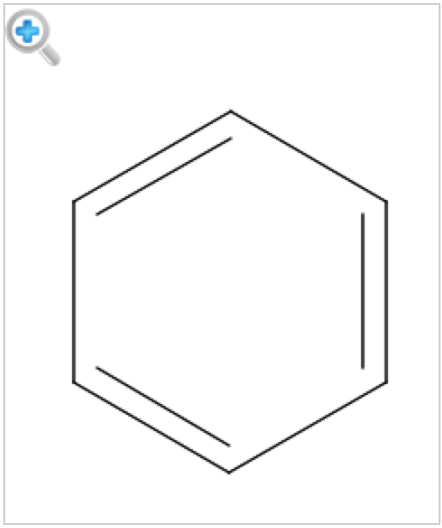
ToxPredict

Estimate toxicological hazard of a chemical structure





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

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