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EPA United States Environmental Protection Agency

US EPA QSAR Prediction and Hazard Comparison Tools

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October 23, 2021

EPA United States Environmental Protection Agency

Outline

- Basics of QSAR modeling
- Tools to estimate toxicity/properties
  - TEST (Toxicity Estimation Software Tool)
  - OPERA (OPEn Structure-activity Relationship App)
  - EPI Suite (EPISUITE Estimation Programs Interface Suite™)
- Tools to compare chemical alternatives
  - HCD (Hazard Comparison Dashboard)

Basics QSAR

- Molecules are converted to numerical representations known as descriptors
- Properties are calculated using equations based on the descriptor values:

$$Toxicity = a_0 + a_1x_1 + a_1x_1 + \ldots a_nx_{n1}$$

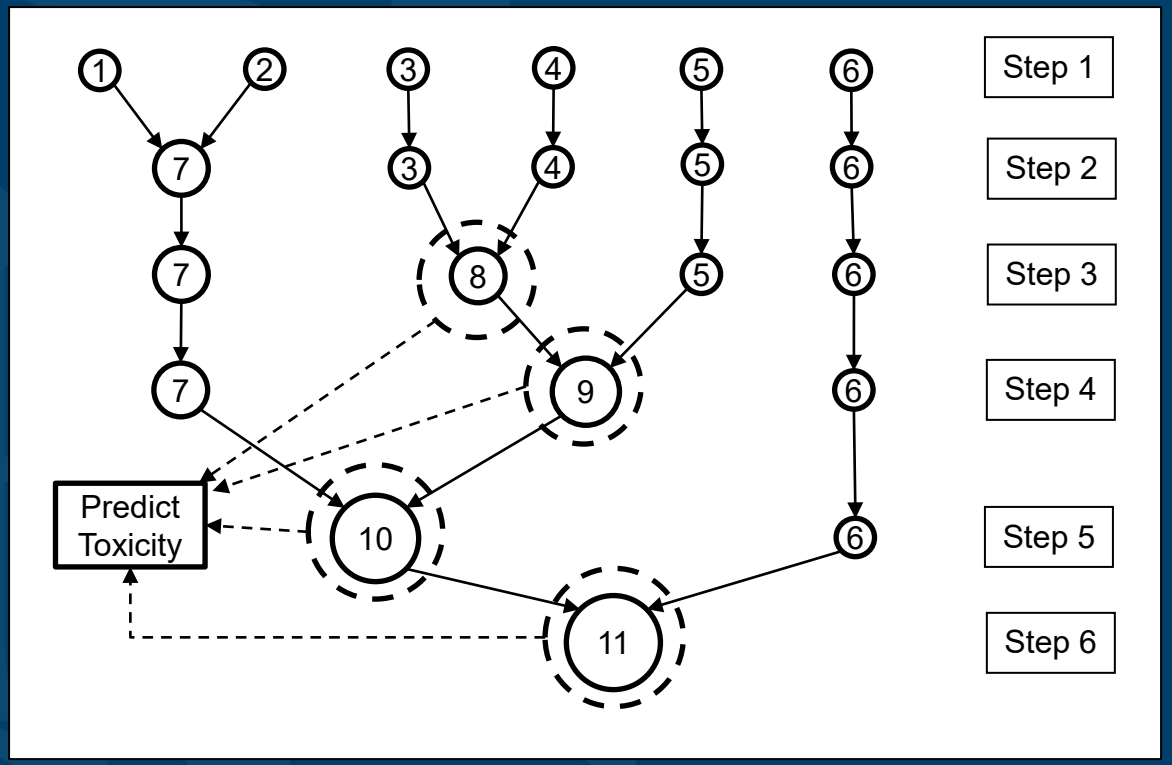
- Overall set is randomly split into a training and prediction set
- Valid predictions must be within a domain of applicability

Methods in TEST 5.1

- There are several QSAR methods available in current TEST software:
  - Hierarchical clustering
  - Single Model
  - Group contribution
  - Nearest neighbor
  - Consensus
- See the TEST User's guide for detailed information

Hierarchical clustering

- Similar chemicals are grouped together but not necessarily on expert defined chemical classes
- Uses structural information from entire data set instead of just from chemicals in SAR



- A prediction is made using the average of the predictions from the MLR models for the closest cluster from each step

Single model

- Predictions is made using multilinear regression model fit to entire training set:

$$Tox = \sum a_i x_i + a_0$$

- Descriptors, x_i, are 2d molecular descriptors
- Example, 48 hr *Daphnia magna* LC_{50} model:
  - Toxicity = 1.2157 × (xc4) + 0.1341 × (StN) + 0.6974 × (SsSH) - 1.3213 × (SsOH_acnt) + 0.8605 × (Hmax) + 1.4685 × (ssi) - 0.9197 × (MDEN33) + 0.2238 × (BEHm1) + 1.4502 × (BEHp1) + 2.4060 × (Mv) + 1.9085 × (MATS1m) - 2.4036 × (MATS1e) - 0.3463 × (GATS3m) + 0.0255 × (AMR) - 1.4215 × (-C(=S)- [2 nitrogen attach]) - 0.7185 × (AN) - 1.0232 × (-N< [attached to P]) - 1.5228 × (-S(=O)(=O)- [aromatic attach]) - 6.5594

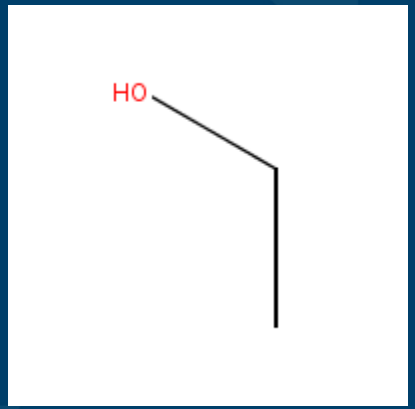
Group contribution

- Predictions is made using multilinear regression model fit to entire training set:

$$Tox = \sum a_i x_i + a_0$$

- Descriptors, x_i, are molecular fragment counts

Descriptor	x_i	a_i	$a_i \times x_i$
-CH3 [aliphatic attach]	1	0.23	0.23
-CH2- [aliphatic attach]	1	0.27	0.27
-OH [aliphatic attach]	1	-0.58	-0.58
Model intercept (a_0)	1	1.96	1.96
Tox (-Log10(LC_{50} mol/L))			1.88

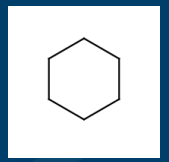
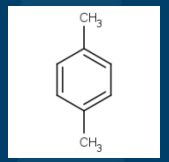


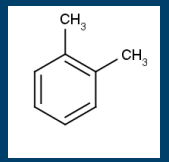
Nearest Neighbor

- Predicted toxicity is simply the average of the three nearest neighbors (i.e. read across)
- The neighbors are those with highest similarity coefficient:

$$SC_{i,k} = \frac{\sum_{j=1}^{\#descriptors} x_{ij} x_{kj}}{\sqrt{\sum_{j=1}^{\#descriptors} x_{ij}^{2} \cdot \sum_{j=1}^{\#descriptors} x_{kj}^{2}}}$$

- All neighbors must exceed a minimum cosine similarity coefficient
- For example the predicted FHM LC_{50} for benzene is made using average of values for



Consensus model

- The consensus prediction is simply the average predicted value for all the models that have predictions inside their applicability domain
- A prediction is made if at least two models have a valid prediction in terms of their respective applicability domain
- Using multiple models minimizes bad predictions and maximizes prediction accuracy
- Using different applicability domains maximizes prediction coverage
- This method is recommended method to use

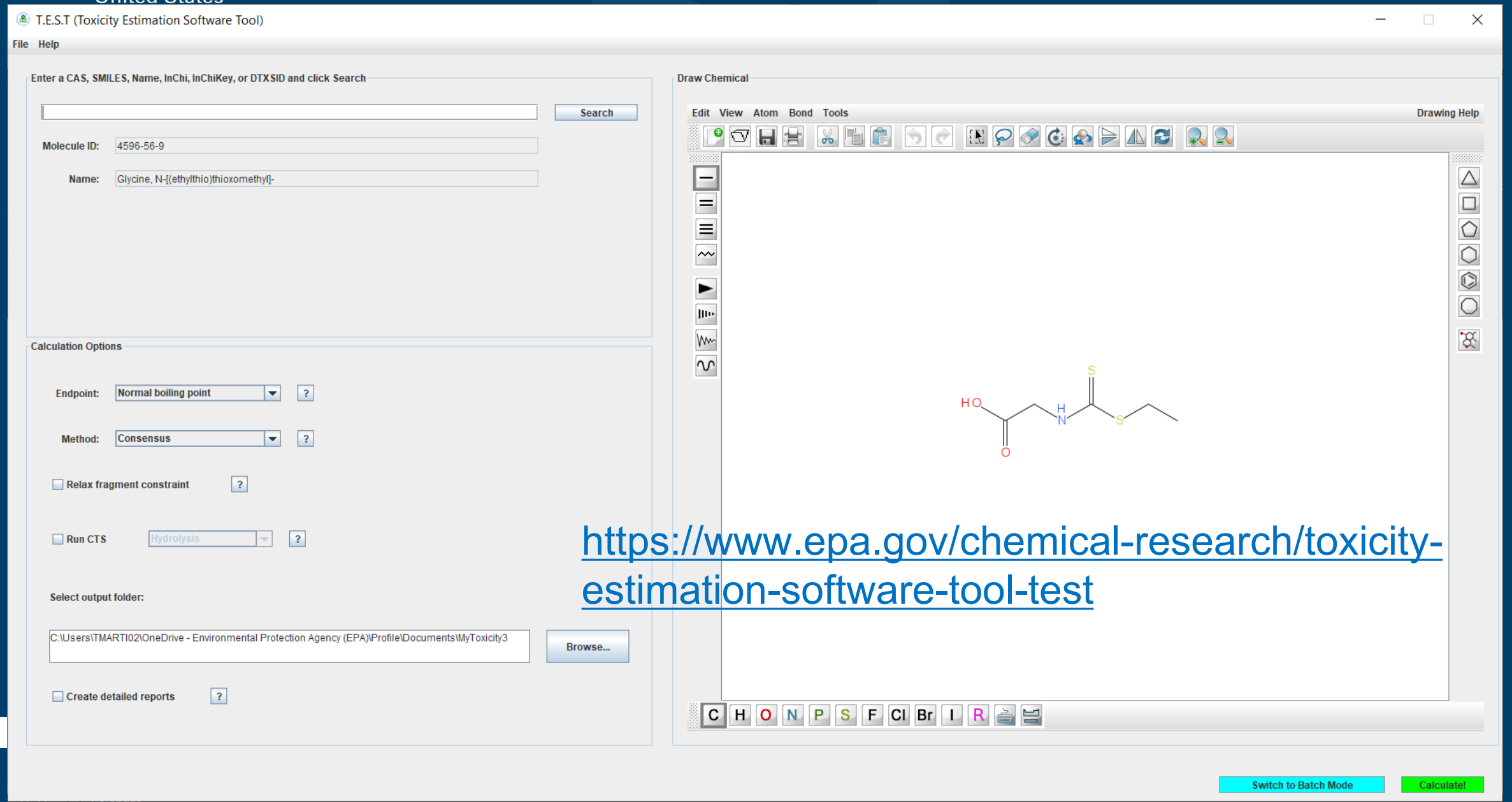
Future Work QSAR Methods

- **Python based QSAR methods**
  - RF - Random Forest
  - SVM – Support Vector Machine
  - DNN – Deep Neural Network
  - XGBoost – eXtreme Gradient Boosting
  - Consensus – average of above methods
- Easily implementable as web services for both model building and model prediction

Ways to access TEST predictions

- Downloadable TEST software
  - https://www.epa.gov/chemical-research/toxicity-estimation-software-tool-test
- WebTEST
  - https://comptox.epa.gov/dashboard/predictions/index
- Stored predictions on the Dashboard
  - https://comptox.epa.gov/dashboard/dsstoxdb/results?search=DTXSID3039242#properties

TEST (Toxicity Estimation Software Tool)



https://www.epa.gov/chemical-research/toxicity-estimation-software-tool-test

WebTEST (real-time predictions)

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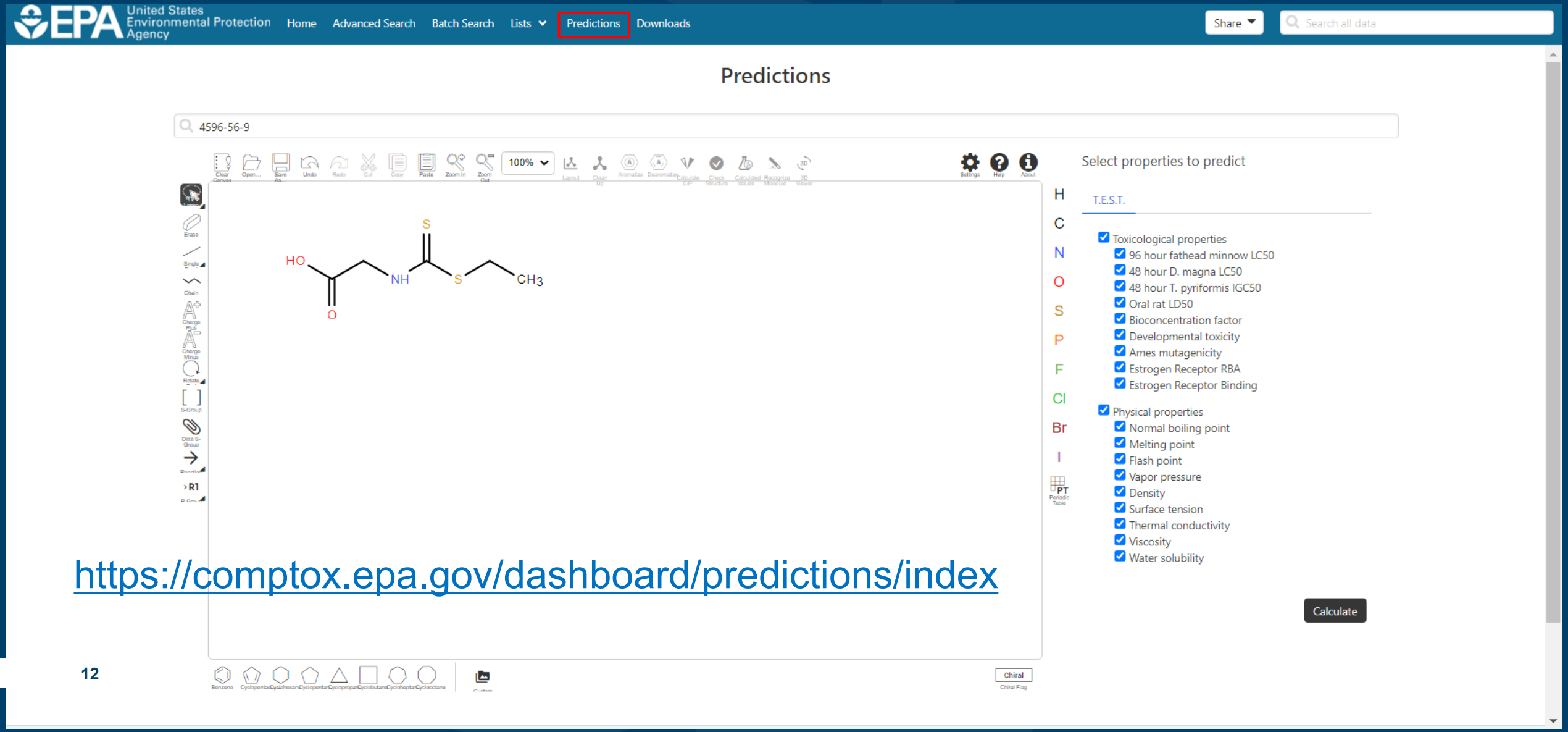

https://comptox.epa.gov/dashboard/predictions/index

Stored Predictions on the Dashboard

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

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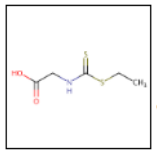
Home | Advanced Search | Batch Search | Lists | Predictions | Downloads | Copy | Share | Submit Comment | Search all data



Glycine, N-[(ethylthio)thioxomethyl]-

4596-56-9 | DTXSID00400783

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
- COMMENTS

Property: Summary

Summary

Download | Columns | Search query

Property	Experimental average	Predicted average	Experimental median	Predicted median	Experimental range	Predicted range	Unit
Water Solubility	8.15e-2 (2)	0.763	8.15e-2	8.11e-2	8.13e-2 to 8.16e-2	2.96e-2 to 2.18	mol/L
Melting Point	-	128		128	-	127 to 130	°C
Flash Point	-	142		142	-	132 to 151	°C
Density	-	1.37		1.37	-	1.34 to 1.40	g/cm^3
Boiling Point	-	311		311	-	296 to 326	°C
LogKow: Octanol-Water	-	0.579		0.599	-	-6.98e-2 to 1.21	-
Surface Tension	-	64.4			-	64.4	dyn/cm
Index of Refraction	-	1.60			-	1.60	-
Molar Refractivity	-	45.7			-	45.7	cm^3
Polarizability	-	18.1			-	18.1	Å^3
Vapor Pressure	-	2.73e-5		2.73e-5	-	9.44e-6 to 4.51e-5	mmHg
Molar Volume	-	133			-	133	cm^3
LogKoa: Octanol-Air	-	7.92			-	7.92	-
Henry's Law	-	1.96e-9			-	1.96e-9	atm-m3/mole

Stored Predictions on the Dashboard

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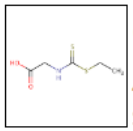
EPA United States Environmental Protection Agency | Home | Advanced Search | Batch Search | Lists | Predictions | Downloads | Copy | Share | Submit Comment | Search all data



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- RELATED SUBSTANCES
- SYNONYMS
- LITERATURE
- LINKS
- COMMENTS

Property

Water Solubility

Water Solubility

Download Summary

Type	Average	Median	Range	Unit
Experimental	8.15e-2	8.15e-2	8.13e-2 to 8.16e-2	mol/L
Predicted	0.763	8.11e-2	2.96e-2 to 2.18	mol/L

Experimental

Download Experimental Data

Source	Result	Experimental Details
PhysPropNCCT	8.16e-2	
Kovdienko, et. al. Molecular informatics 29.5 (2010): 394-406.	8.13e-2	

Predicted

Download Predicted Data

Source	Result	Calculation Details	QMRF
TEST	2.96e-2	TEST Report	Not Available
ACD/Labs	2.18	Not Available	Not Available
OPERA	8.11e-2	OPERA Model Report [Inside AD]	Available

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TEST Report

Predicted Water solubility at 25Â°C for 4596-56-9 from Consensus method

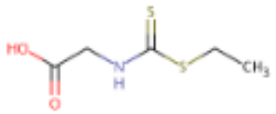
Prediction results

Endpoint	Experimental value (CAS= 4596-56-9) Source: EPI Suite v 4.00	Predicted value[a]
Water solubility at 25Â°C -Log10(mol/L)	1.09	1.53
Water solubility at 25Â°C mg/L	14606.83	5316.84

[a]Note: the test chemical was present in the external test set.

Individual Predictions

Method	Predicted value -Log10(mol/L)
Hierarchical clustering	1.36
Group contribution	1.92
Nearest neighbor	1.31

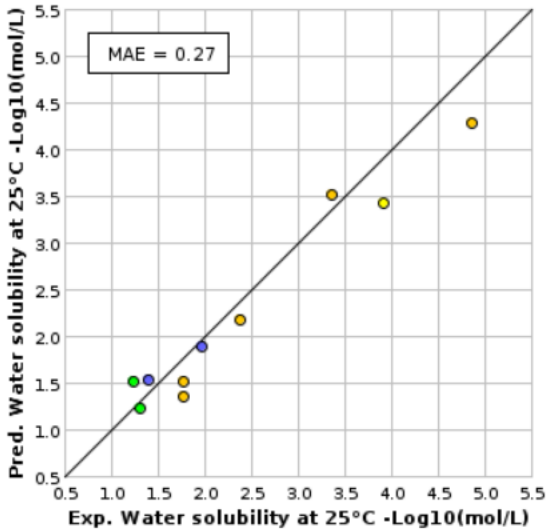


TEST Report, cont.

Predictions for the test chemical and for the most similar chemicals in the training set

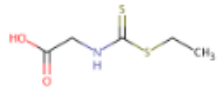
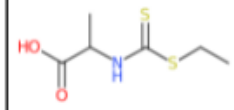
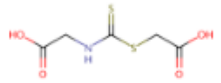
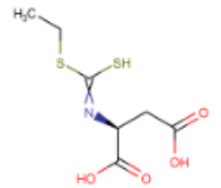
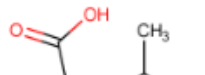
If the predicted value matches the experimental values for similar chemicals in the training set (and the similar chemicals w value.

Prediction results (colors defined in table below)



Chemicals	MAE*
Entire set	0.50
Similarity coefficient ≥ 0.5	0.27

*Mean absolute error in -Log10(mol/L)

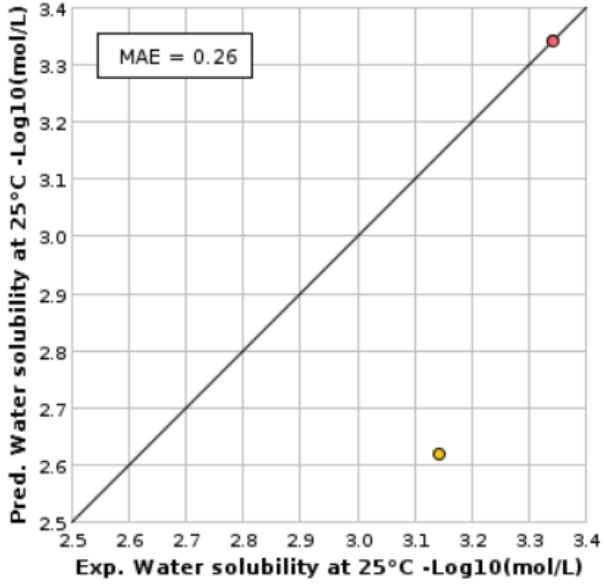
CAS	Structure	Similarity Coefficient	Experimental value -Log10(mol/L)	Predicted value -Log10(mol/L)
4596-56-9 (test chemical)			1.09	1.53
70561-60-3		0.97	1.23	1.52
29677-65-4		0.90	1.30	1.23
5139-67-3		0.82	1.39	1.54
				

TEST Report, cont.

Predictions for the test chemical and for the most similar chemicals in the external test set

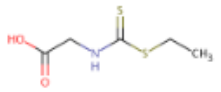
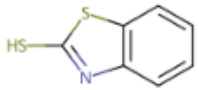
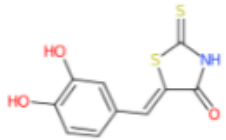
If the predicted value matches the experimental values for similar chemicals in the test set (and the similar chemicals were

Prediction results (colors defined in table below)



Chemicals	MAE*
Entire set	0.58
Similarity coefficient ≥ 0.5	0.26

*Mean absolute error in -Log10(mol/L)

CAS	Structure	Similarity Coefficient	Experimental value -Log10(mol/L)	Predicted value -Log10(mol/L)
4596-56-9 (test chemical)			1.09	1.53
149-30-4		0.65	3.14	2.62
97852-89-6		0.51	3.34	3.34

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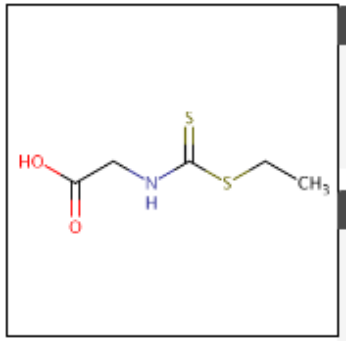
OPERA Prediction Report

OPERA Models: Water Solubility

Glycine, N-[(ethylthio)thioxomethyl]-

4596-56-9 | DTXSID00400783

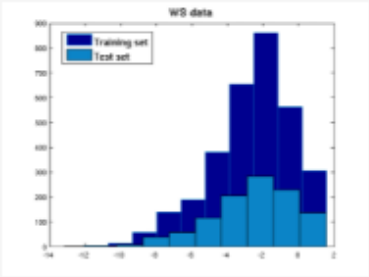
Print PDF

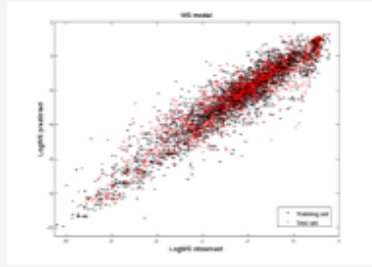


Model Results

Predicted value: 8.11e-2 mol/L
Global applicability domain: Inside
Local applicability domain index: 0.998
Confidence level: 0.859

Model Performance



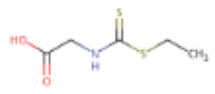


QMRF

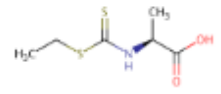
Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.870	0.810	0.870	0.820	0.860	0.860

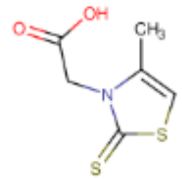
Nearest Neighbors from the Training Set



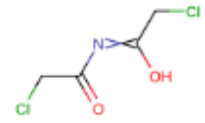
Glycine, N-[(ethylthio)thioxomethyl]-
Measured:0.0816206
Predicted: 0.08



L-Alanine, N-[(ethylthio)thioxomethyl]-
Measured:0.0798362
Predicted: 0.08



3(2H)-Thiazoleacetic acid, 4-methyl-2-thioxo-
Measured:0.0108843
Predicted: 0.01



Acetamide, 2-chloro-N-(chloroacetyl)-
Measured:0.00588301
Predicted: 0.01

OPERA QMRF

	*QMRF identifier (JRC Inventory):* **Q17-12-0021**
	QMRF Title: OPERA-**model for** Boiling point
	Printing Date: **Oct 17, 2017**

1.QSAR identifier

1.1.QSAR identifier (title):

OPERA-model for Boiling point

1.2.Other related models:

No related models

1.3.Software coding the model:

OPERA V1.5

OPERA (OPEn (quantitative) structure-activity Relationship Application) is a standalone free and open source command line application. It provides a suite of QSAR models to predict physicochemical properties and environmental fate of organic chemicals based on PaDEL descriptors. It is available for download in Matlab, C and C++ languages from github under MIT license.

Kamel Mansouri (mansourikamel@gmail.com)

https://github.com/kmansouri/OPERA.git

PaDEL descriptors V2.21

Open source software to calculate molecular descriptors and fingerprints.

Chun Wei Yap (phayapc@nus.edu.sg)

http://padel.nus.edu.sg/software/padeldescriptor

Alternatives Assessment

- Goal: identify safer alternatives for chemicals of concern.
  - Comparative Chemical Hazard Assessment
  - Exposure Assessment and Life Cycle Assessment

Purpose of the Hazard Comparison Dashboard

- An OECD* review identified gaps including
  - a need for improved access to "automated tools and methods to reduce hours of highly technical work"

- The Hazard Comparison Dashboard aims to fill this gap
  - Display compiled chemical hazard data and enable users to readily compare alternatives

*Organization for Economic Cooperation and Development (OECD) (2013), *Current Landscape of Alternatives Assessment Practice: A Meta-Review.*

Hazard categories

- Scores of Low, Medium, High, and Very High (L, M, H, VH) for:
  - Human Health
    - Acute mammalian toxicity*
    - Carcinogenicity
    - Mutagenicity*
    - Endocrine disruption*
    - Reproductive toxicity
    - Developmental toxicity*
    - Neurotoxicity
    - Systemic toxicity
    - Skin sensitization
    - Skin irritation
    - Eye irritation
  - Ecotoxicity
    - Acute aquatic toxicity*
    - Chronic aquatic toxicity
  - Fate
    - Persistence
    - Bioaccumulation*

***Six endpoints can be predicted using Quantitative Structure-Activity Relationship (QSAR) models in WebTEST**

Sources of Hazard Data

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- **GHS H-codes**
  - Safe Work Australia Hazardous Chemical Information System (HCIS)
  - Canada CNESST Workplace Hazardous Materials Information System (WHMIS)
  - European Chemicals Agency (ECHA) Classification Labeling and Packaging (CLP)
  - National Institute of Technology and Evaluation (NITE) of Japan
  - Ministry of Human Resources Malaysia Industry Code of Practice on Chemicals Classification and Hazard Communication
- **Hazard categories**
  - Germany Permanent Senate Commission for the Investigation of Health Hazards of Chemical Compounds in the Work Area (MAK Commission)
  - New Zealand Environmental Protection Authority
- **Quantitative toxicity data**
  - ChemID*plus, ToxVal v8*
- **Quantitative Structure-Activity Relationships (QSAR) Predictions**
  - WebTEST, OPERA
  - Ministry of Environment and Food of Denmark Advisory List for Self-Classification of Dangerous Substances

Sources of Hazard Data

- **Hazardous Chemical Lists**
  - Environment and Climate Change Canada Domestic Substance List (DSL)
  - EPA mid-Atlantic Region Human Health Risk-Based Concentrations
  - Health Canada Priority Substance Lists (Carcinogenicity and Reproductive Tox)
  - International Agency for Research on Cancer (IARC) Monographs
  - Integrated Risk Information System (IRIS)
  - National Institute for Occupational Safety and Health (NIOSH) list of potential occupational carcinogens
  - California Proposition 65
  - ECHA Registration, Evaluation, Authorization and Restriction of Chemicals (REACH) Candidate List of Substances of Very High Concern for Authorization
  - Report On Carcinogens
  - Chemsec Substitute It Now (SIN) List
  - The Endocrine Disruption Exchange (TEDX) List of Potential Endocrine Disruptors
  - Toxic Substances Control Act (TSCA) Work Plan
  - University of Maryland (UMD) List of Acute Toxins, Teratogens, Carcinogens, or Mutagens

Criteria for converting acute mammalian toxicity data into hazard scores

Source	Endpoint	Score				
		VH	H	M	L	N/A
DfE criteria	Oral LD50 (mg/kg)	≤ 50	> 50 - 300	> 300 - 2000	> 2000	
	Hazard Code	H300	H301	H302		
ChemIDplus; T.E.S.T. Predicted*	Oral LD50* (mg/kg)	≤ 50	> 50 - 300	> 300 - 2000	> 2000	
Australia; Canada; ECHA CLP; Japan**; Malaysia	Hazard Code	H300	H301	H302	H303	
Denmark	Category	AcuteTox1 and AcuteTox2	AcuteTox3	AcuteTox4		
New Zealand	Category	Category 6.1A	Category 6.1C	Category 6.1D	Category 6.1E	
		Category 6.1B				
TSCA Work Plan			Acute mammalian toxicity			
UMD		Acute toxin				

*T.E.S.T. Predicted predicts rat LD50 values. ChemIDplus LD50 values for rats, mice, rabbits, and guinea pigs were included.
**Japan is the only source that included H303.

Assigning the Overall Score

- Trumping Method: **overall score is the most toxic score from the most authoritative source**

1. Authoritative (e.g., ECHA CLP)
2. Screening (e.g., ChemIDplus)
3. Predicted (e.g., WebTEST)

Data coverage for the active non-confidential portion of the TSCA inventory (n = 18,696)

Endpoint	% Coverage*
Acute Mammalian Toxicity Oral	18.5%
Acute Mammalian Toxicity Inhalation	6.7%
Acute Mammalian Toxicity Dermal	8.6%
Carcinogenicity	3.6%
Genotoxicity Mutagenicity	9.6%
Endocrine Disruption	2.3%
Reproductive	3.4%
Developmental	4.1%
Neurotoxicity Repeat Exposure	1.5%
Neurotoxicity Single Exposure	1.9%
Systemic Toxicity Repeat Exposure	5.6%
Systemic Toxicity Single Exposure	5.0%
Skin Sensitization	3.6%
Skin Irritation	12.3%
Eye Irritation	13.1%
Acute Aquatic Toxicity	40.3%
Chronic Aquatic Toxicity	9.4%
Persistence	40.4%
Bioaccumulation	40.1%

* Omits QSAR predictions from T.E.S.T. and Denmark

EPA United States Environmental Protection Agency

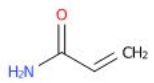
Hazard Comparison Dashboard

version: UAT, build: 2021-09-01 04:38:23 UTC

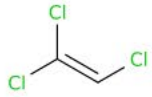
HAZARD | PREDICT | SEARCH | STANDARDIZE | TOXPRINT

No Metabolites | No Analogs

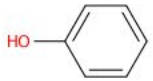
10 / 10



Acrylamide
79-06-1



Trichloroethylene
79-01-6



Phenol
108-95-2

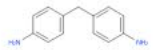
Formaldehyde
50-00-0

Glutaraldehyde
111-30-8

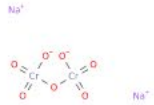
Hydrazine
302-01-2

Ethylene oxide
75-21-8

Hydrazine hydr...
7803-57-8



4,4'-Diaminobip...
101-77-9



Sodium dichro...
10588-01-9

Sample Web HCD Output

Toxicity: VH - Very High H - High M - Medium L - Low I - Inconclusive N/A - Not Applicable *Authority:* **Authoritative** Screening *QSAR Model*

Skipped (0)
Unlikely (0)
Filters (0)
Sorting (0)
Structure

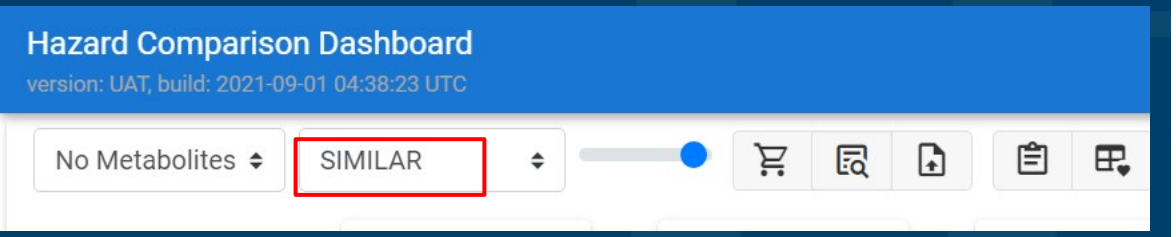
CAS / Name	Human Health Effects															Ecotoxicity		Fate	
	Acute Mammalian Toxicity							Neurotoxicity		Systemic Toxicity									
	Oral	Inhalation	Dermal	Carcinogenicity	Genotoxicity Mutagenicit	Endocrine Disruption	Reproductive	Developmental	Repeat Exposure	Single Exposure	Repeat Exposure	Single Exposure	Skin Sensitization	Skin Irritation	Eye Irritation	Acute Aquatic Toxicity	Chronic Aquatic Toxicity	Persistence	Bioaccumulation
79-06-1 Acrylamide	H	M	M	VH	VH	*L*	M	H	H	H	H	H	H	H	H	M	M	L	L
79-01-6 Trichloroethylene	L	M	L	VH	VH	*I*	H	H	H	H	H	M	H	H	H	H	VH	H	L
108-95-2 Phenol	H	H	H	H	H	H	H	H	H	H	M	H	H	VH	VH	H	H	L	H
50-00-0 Formaldehyde	H	H	H	VH	H	H		L			L	M	H	VH	VH	H	L	L	L
111-30-8 Glutaraldehyde	H	VH	H	M	VH	H	H	L		H	H	M	H	VH	VH	VH	H	L	L
302-01-2 Hydrazine	H	H	H	VH	VH		H	M	H	H	H	H	H	VH	VH	VH	VH	L	L
75-21-8 Ethylene oxide	VH	H	I	VH	VH	H	H	H	H	H	H	M	H	H	H	M	L	H	L
7803-57-8 Hydrazine hydrate...	VH	VH	VH	VH	VH		M	I	H	H	H	H	H	VH	VH	VH	VH		
101-77-9 4,4'-Diaminobiphe...	H	I	VH	VH	H	L	I	*H*		H	M	H	H	L	H	VH	H	L	L
10588-01-9 Sodium dichromate	H	VH	M	VH	VH		H	H			H	H	H	VH	VH	VH	VH	H	L

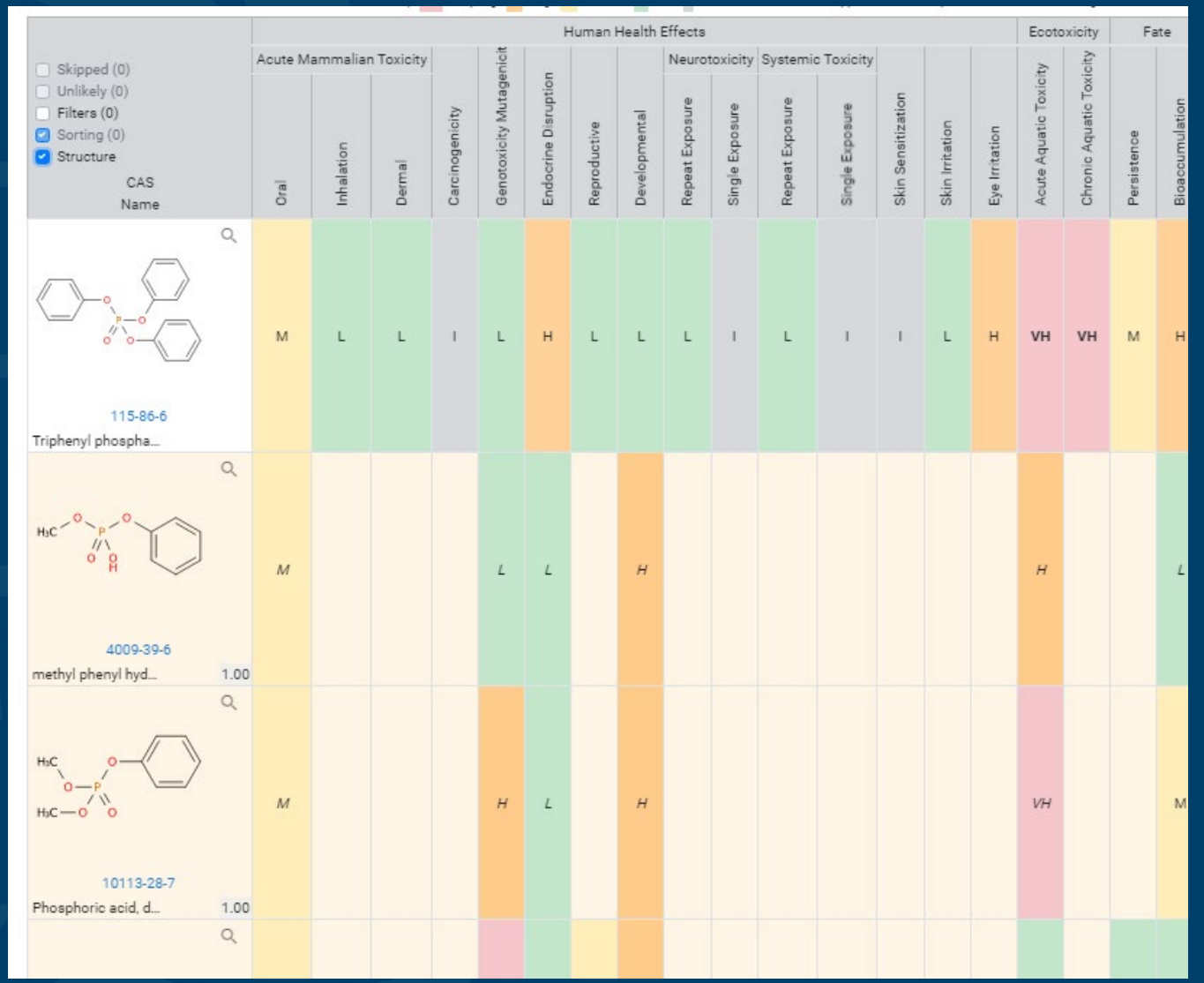
HCD Results with CTS* transformations

https://qed.epa.gov/cts/

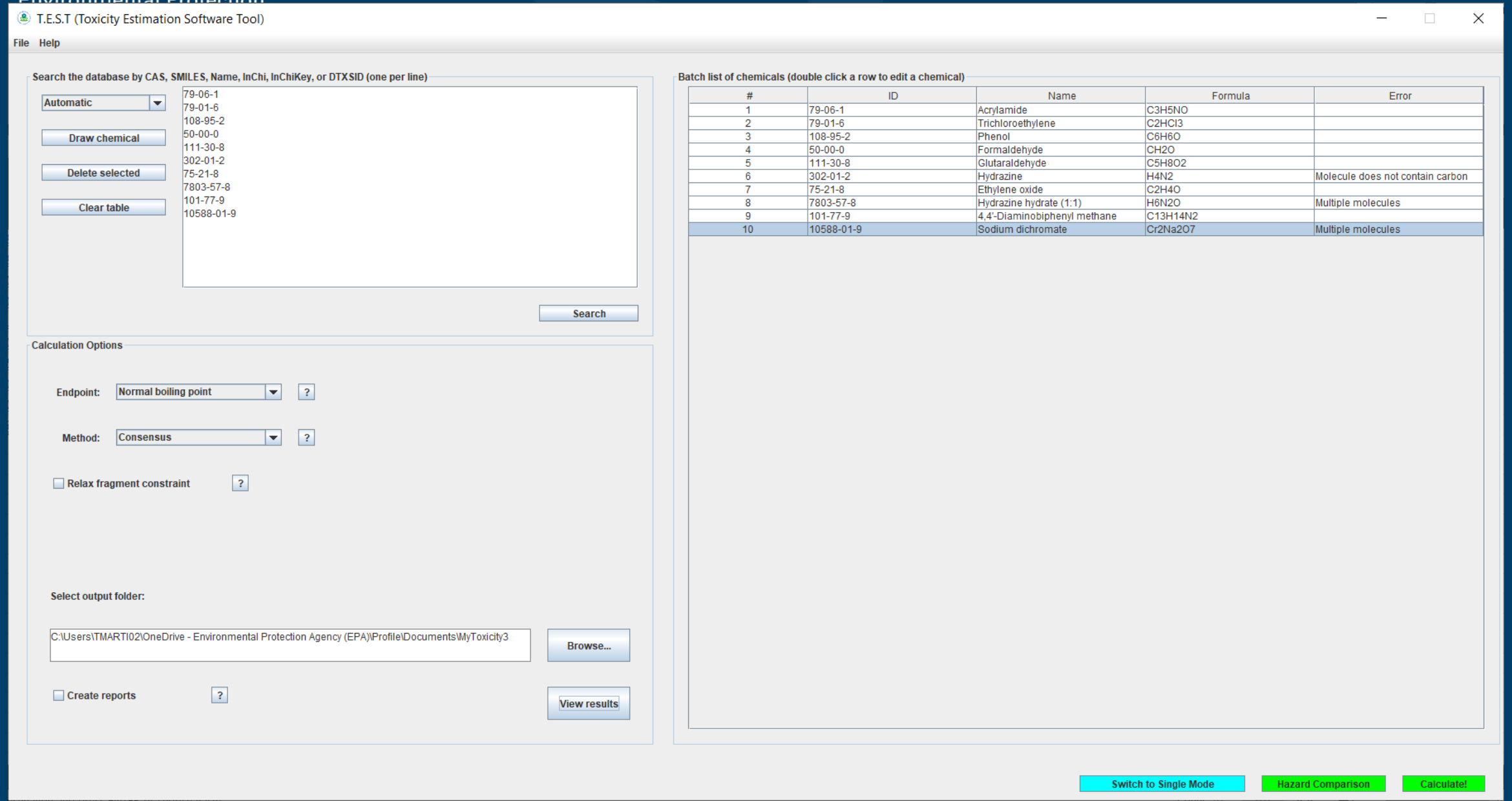
* Chemical Transformation Simulator generates breakdown products via environmental and biological transformation pathways

HCD with analog search





Batch mode of TEST



Sample Hazard Comparison Output in TEST

Hazard comparison

Final Scores | Score Records | Score Records Exposure 79-06-1

CAS	Name	Acute Mammalian Toxicity Oral	Acute Mammalian Toxicity Inhalation	Acute Mammalian Toxicity Dermal	Skin Sensitization	Skin Irritation	Eye Irritation	Carcinogenicity	Genotoxicity Mutagenicity	Endocrine Disruption	Reproductive	Developmental	Neurotoxicity Repeat Exposure	Neurotoxicity Single Exposure	Systemic Toxicity Repeat Exposure	Systemic Toxicity Single Exposure	Acute Aquatic Toxicity	Chronic Aquatic Toxicity	Persistence	Bioaccumulation	Exposure
79-06-1	Acrylamide	H	M	M	H	H	H	VH	VH	L	M	H	H	H	H	H	M	M	L	L	H
79-01-6	Trichloroet...	L	M	L	H	H	H	VH	VH	L	H	H	H	H	H	M	H	VH	H	L	H
108-95-2	Phenol	H	H	H	H	VH	VH	H	H	H	H	H	H	H	M	H	H	H	L	H	VH
50-00-0	Formaldeh...	H	H	H	H	VH	VH	VH	H	H		L			L	M	H	L	L	L	H
111-30-8	Glutaralde...	H	VH	H	H	VH	VH	M	H	H	H	L		H	H	M	VH	H	L	L	H
302-01-2	Hydrazine	H	H	H	H	VH	VH	VH	VH		H	M	H	H	H	H	VH	VH	L	L	
75-21-8	Ethylene o...	VH	H	I	H	H	H	VH	VH	H	H	H	H	H	H	M	M	L	H	L	VH
7803-57-8	Hydrazine ...	VH	VH	VH	H	VH	VH	VH	VH		M	I	H	H	H	H	VH	VH		I	
101-77-9	4,4'-Diami...	H	I	VH	H	L	H	VH	H	L	I	H		H	M	H	VH	H	L	L	H
10588-01-9	Sodium di...	H	VH	M	H	VH	VH	VH	VH		H	H			H	H	VH	VH	H	L	

Score Record Output in TEST

Hazard comparison

Final Scores | Score Records | Score Records Systemic Toxicity Repeat Exposure 79-06-1

CAS	name	hazardName	source	sourc...	listType	score	rationale	route	category	hazardCode	hazardStat...	note	note2	toxvalID	testOrganis...	testType	valuel
79-06-1	acrylamide;...	Systemic T...	ECHA CLP		Authoritative	H	Score of H was assigned based on a hazard code of H372		STOT RE 1	H372	Causes da...						
79-06-1	Acrylamide	Systemic T...	Australia		Screening	H	Score of H was assigned based on a hazard code of H372		Specific tar...	H372	Causes da...	N (The clas...					
79-06-1	Acrylamide	Systemic T...	Canada		Screening	H	Score of H was assigned based on a hazard code of H372		Specific tar...	H372	Causes da...	Comments...					
79-06-1	Acrylamide	Systemic T...	Japan		Screening	H	Score of H was assigned based on a hazard code of H372		Category 1 ...	H372	Causes da...	As for hum...					
79-06-1	Acrylamide;...	Systemic T...	Malaysia		Screening	H	Score of H was assigned based on a hazard code of H372		STOT RE 1	H372	Causes da...						
79-06-1	Acrylamide	Systemic T...	New Zeala...		Screening	H	Score was assigned based on a category of Category 6.9A (Category ...	dermal	Category 6....		Toxic to hu...	EndPoint: <...					
79-06-1	Acrylamide	Systemic T...	New Zeala...		Screening	H	Score was assigned based on a category of Category 6.9A (Category ...	inhalation	Category 6....		Toxic to hu...	EndPoint: <...					
79-06-1	Acrylamide	Systemic T...	New Zeala...		Screening	H	Score was assigned based on a category of Category 6.9A (Category ...	oral	Category 6....		Toxic to hu...	EndPoint: <...					
79-06-1	Acrylamide	Systemic T...	ToxVal v8	ECHA	Screening	H	2 year Oral NOAEL < 1.25 mg/kg-day	oral						67861	rat	NOAEL	=
79-06-1	Acrylamide	Systemic T...	ToxVal v8	HPVIS	Screening	H	1 month Oral NOAEL < 30.0 mg/kg-day	oral						667461	rat	NOAEL	=
79-06-1	Acrylamide	Systemic T...	ToxVal v8	HPVIS	Screening	H	3 months Oral NOAEL < 10.0 mg/kg-day	oral						667462	rat	NOAEL	=
79-06-1	Acrylamide	Systemic T...	ToxVal v8	HPVIS	Screening	H	3 months Oral NOAEL < 10.0 mg/kg-day	oral						667463	rat	NOAEL	=
79-06-1	Acrylamide	Systemic T...	Australia		Screening	M	Score of M was assigned based on a hazard code of H373		Specific tar...	H373	May cause ...	N (The clas...					

Strengths and Limitations of the Hazard Comparison Dashboard

- Strengths
  - Provides rapid way to compare chemicals and retrieve hazard data
  - Includes data from several sources including QSAR models

- Limitations
  - Data gaps
  - Automation limits the scope of data searching and quality assurance, particularly of primary sources

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Future Research Needs

- Update the data from each source

- Add additional data sources into the AA Dashboard
  - QSAR models for additional endpoints
  - Quantitative data from REACH dossiers

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Questions???

The views expressed in this presentation are those of the author and do not necessarily represent the views or policies of the U.S. Environmental Protection Agency