US EPA CompTox Chemistry Dashboard as a source of data to fill data gaps for chemical sources of risk

Antony Williams¹, Chris Grulke¹, Kamel Mansouri⁴, Kathie Dionisio², Katherine Phillips², Grace Patlewicz¹, Imran Shah¹, Kristin Isaacs², Todd Martin³, John Wambaugh¹, Ann Richard¹ and Richard Judson¹

National Center for Computational Toxicology, U.S. Environmental Protection Agency, RTP, NC
 National Exposure Research Laboratory, U.S. Environmental Protection Agency, RTP, NC
 National Risk Management Research Laboratory, U.S. Environmental Protection Agency, Cincinnati, OH
 Scitovation, RTP, NC

The views expressed in this presentation are those of the author and do not necessarily reflect the views or policies of the U.S. EPA

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- The Chemistry Dashboard went online on April 1st 2016
- Initial concept was as an integration hub for NCCT chemistry data
- Two years later, with 10k users a month, it is fulfilling the promise with an underlying architecture for integrating CompTox data
- Hazard and Exposure data to fill data gaps

The CompTox Chemistry Dashboard



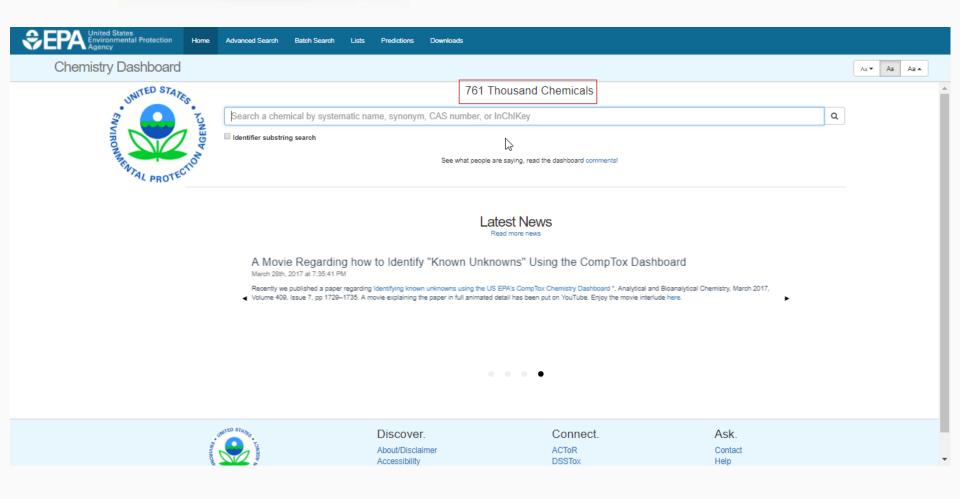
• A publicly accessible website delivering access:

- ~760,000 chemicals with related property data
- Experimental and predicted physicochemical property data
- Experimental Human and Ecological hazard data
- Integration to "biological assay data" for 1000s of chemicals
- Information regarding consumer products containing chemicals
- Links to other agency websites and public data resources
- "Literature" searches for chemicals using public resources
- "Batch searching" for thousands of chemicals
- Real time prediction of physchem and toxicity endpoints

CompTox Chemistry Dashboard



https://comptox.epa.gov/dashboard



Detailed Chemical Pages



Chemistry Dashboa	n Home Adva	nced Search	Batch Search							_		
Chemistry Dashboa			batch Search	Lists	Predictions	Downloads				s	earch All Data	Q
-	rd EPAHFR							Submit Comme	nt Copy	• A	a▼ Aa	Aa 🔺
•	ylene gly						\$					
	ox_Substance_Id: Found	1 result for 'DT	XSID0021206'.									
			Wikipedia									
	он І		C3H8O2. It is is classed as a	a viscous co a diol and is	olorless liquid whi miscible with a b	ch is nearly ode road range of s	thetic organic compou orless but possesses i olvents, including wat duction of polymers, b	a faintly sweet tast er, acetone, and cl	e. Chemically it nloroform. It is	t		
HO	$\mathbf{\mathbf{\mathbf{\mathbf{\mathbf{\mathbf{\mathbf{\mathbf{\mathbf{\mathbf{\mathbf{\mathbf{\mathbf{\mathbf{\mathbf{\mathbf{\mathbf{\mathbf{$		Intrinsic Prop	perties								
	C	H ₃	Structural Id	entifiers								
			Linked Subs	tances								
			Presence in	Lists								
			Record Infor	mation								
			Quality Cont	trol Notes								
Chemical Properties Env. Fate/Transpo	ort Hazard AD	ME (Beta)	Exposure	Bioassays	Similar Com	pounds R	elated Substances	Synonyms	Literature	Links	Comment	5

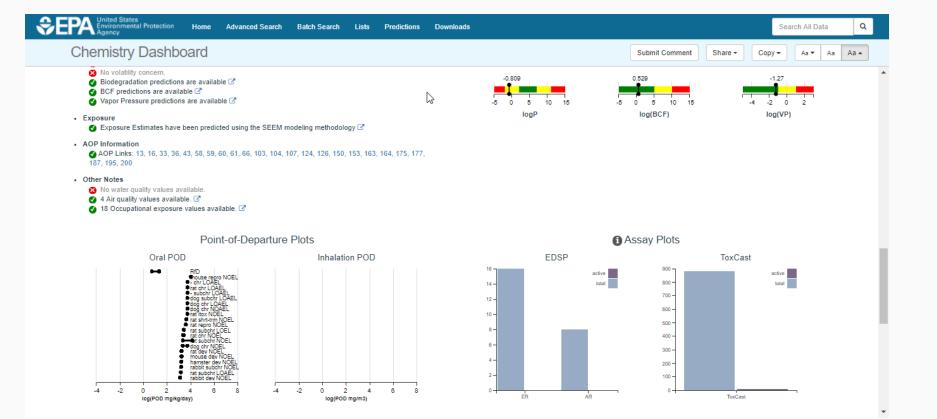
The Executive Summary (NEW)



EPA Control of the states of t	ads			Searc	h All Data		۹
Chemistry Dashboard		Submit Comment	Share +	Сору 🕶	Aa 🔻 🗛	a Aa	•
Executive S	ummary						
 Quantitative Risk Assessment Values No IRIS values PPRTV values available C[*] EPA RSL values available C[*] Minimum RfD: 5.0 mg/kg-day (subchronic, PPRTV (ORNL), oral, 8) C[*] Minimum RfC: 0.028 mg/m3 (subchronic, RAIS, inhalation, 7) C[*] IVIVE POD not calculated 							
Quantitative Hazard Values ✓ Minimum oral POD: 1.2e+3 mg/kg-day (developmental, COSMOS, oral, 3) So inhalation POD values Lowest Observed Bioactivity Equivalent Level: NR1H4		ional Screening					
Cancer Information No cancer slope factor	Class screening level (residential Soil) (mg/kg-day)		THQ THQ=1	Value 13000	00	-	
 No inhalation unit risk value Carcinogenicity data available: EPA OPP cancer class: E University of Maryland carcinogenicity warning; 	screening level (residential Soil) (mg/kg-day)		THQ=0.1	13000	0		
Image: Second	screening level (industrial soil) (mg/kg-day)		THQ=1	16000	000		
Reproductive Toxicology	screening level (industrial soil) (mg/kg-day)		THQ=0.1	16000)0		
	screening level (tap water) (ug/L)		THQ=1	40000)		
 Chronic Toxicology 25 Chronic toxicity PODs available I 	screening level (tap water) (ug/L)		THQ=0.1	40000			
Subchronic Toxicology	GIABS (mg/kg-day)		-	1			
	ABS (mg/kg-day)		-	0.1		1	
 Developmental Toxicology ✓ 5 Developmental toxicity PODs available ^C[*] 	risk-based SSL (mg/m3)		THQ=1	81		1	
Acute Toxicology	risk-based SSL (mg/m3)		THQ=0.1	8.1			
	RfDo (mg/kg-day)		-	20			

The Executive Summary (NEW)





The Executive Summary (NEW)





Properties, Fate and Transport

€PA nited States Environmental Protection Agency

Chemistry Da	shboard					Submit	Comment Share - C	Copy → Aa ◆ Aa
Summary		5 1 005						
LogP: Octanol-Water	Download as: TSV -	Excel - SDF -						
Water Solubility	Property	Ave	erage	Med	ian		Range	Unit
Density		Experimental	Predicted	Experimental	Predicted	Experimental	Predicted	
Density	LogP: Octanol-Water	-0.920 (1)	-0.983 (5)	-	-0.966	-0.920	-1.34 to -0.780	-
Flash Point	Water Solubility	13.1 (1)	12.6 (4)	-	11.2	13.1	4.32 to 23.6	mol/L
Melting Point	Density	-	1.02 (2)	-	1.02	-	1.01 to 1.04	g/cm^3
	Flash Point	-	88.8 (2)	-	88.8	-	70.4 to 107	°C
Boiling Point	Melting Point	-60.0 (6)	-30.6 (4)	-60.0	-29.3	-60.0	-42.4 to -21.6	°C
Surface Tension	Boiling Point	187 (6)	180 (5)	187	185	187 to 188	155 to 200	°C
The second construction the	Surface Tension	-	35.5 (2)	-	35.5	-	33.1 to 38.0	dyn/cm
Thermal Conductivity	Thermal Conductivity	-	185 (1)	-	÷	-	-	mW/(m*K)
Vapor Pressure	Vapor Pressure	1.29e-01 (1)	1.91e-01 (4)	-	2.08e-01	1.29e-01	5.37e-02 to 2.95e-01	mmHg
Viscosity	Viscosity	-	12.6 (1)	-	-	-	-	cP
	LogKoa: Octanol-Air	-	6.74 (1)	-	-	-	-	-
LogKoa: Octanol-Air	Henry's Law	-	6.02e-08 (1)	-	-	-	-	atm-m3/mole
Henry's Law	Index of Refraction	-	1.43 (1)	-	-	-	-	-
	Molar Refractivity	-	19.0 (1)	-	-	-	-	cm^3
Index of Refraction	Molar Volume	-	73.4 (1)	-	-	-	-	cm^3
Molar Refractivity	Polarizability	-	7.52 (1)	-	-	-		Å^3

Properties, Fate and Transport

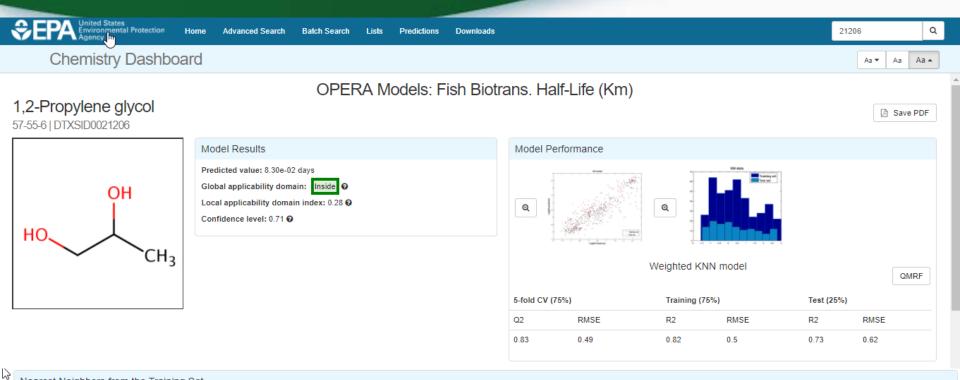


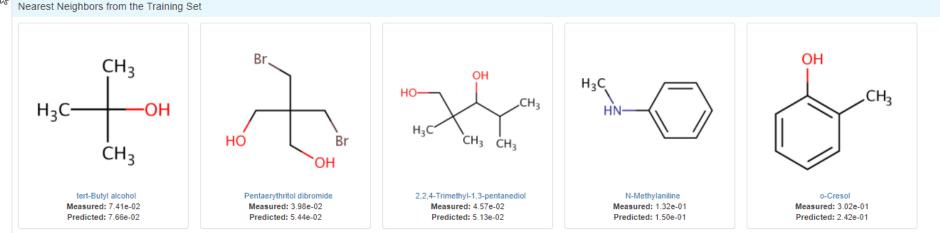
• When we don't have experimental data we predict it...

Property	Average						
	Experimental	Predicted					
Soil Adsorp. Coeff.	2.29 (1)	1.94 (2)	-				
Atmos. Hydroxylation Rate	1.20e-11 (1)	1.30e-11 (1)	-				
Biodeg. Half-Life	-	4.28 (1)	-				
Fish Biotrans. Half-Life (Km)	-	8.30e-02 (1)	-				
Bioaccumulation Factor	-	8.96e-01 (1)	-				
Bioconcentration Factor	-	2.13 (5)	-				

Model Performance Details

United States Environmental Protection Agency





OPERA: OPEN Data and OPEN Models

Mansouri et al. J Cheminform (2018) 10:10 https://doi.org/10.1186/s13321-018-0263-1

Journal of Cheminformatics

RESEARCH ARTICLE



Open Access

vironmental Protection

OPERA models for predicting physicochemical properties and environmental fate endpoints

Kamel Mansouri^{1,2,3*}^(D), Chris M. Grulke¹, Richard S. Judson¹ and Antony J. Williams¹

Access to Chemical Hazard Data



	States mental Protei	ction	Home	Advanced Search	Batch Searc	h Lists	Predictions	Downloads	5			Search All Da	ta
Chemistry	Dashbo	oard	EPAH	FR						Submit Comn	Copy •	Aa 🕶 🗛	Aa
Chemical Properties	Env. Fate/Trar	nsport	Hazard	ADME (Beta)	Exposure	Bioassays	Similar Com	pounds	Related Substance	s Synonyms	Literature	Links Comme	nts
Exposure Limit		Downloa	d table as:	TSV Excel			Huma	an Eco					
Lethality Effect Level Point of Departure			Priorit	¢ ț∳	Subtype	Risk Assessmer Class	t Values	Units 🍦		Exposure Route Specie	es 🗘 Subsourd	e Source	
Toxicity Value		+	8	NOEL	Cardiova	subchronic	5000.0	mg/kg-day	subchronic	oral r	at Vaille et	PPRTV (•
		+	8	NOEL	Endocrine	subchronic	5000.0	mg/kg-day	subchronic	oral r	at Vaille et	PPRTV (L
		+	8	LOEL	Hematol	subchronic	2500.0	mg/kg-day	subchronic	oral r	at Vaille et	PPRTV (
		+	8	LOEL	Hepatic	subchronic	2500.0	mg/kg-day	subchronic	oral r	at Vaille et	PPRTV (
		+	8	NOEL	Immune	immunot	5000.0	mg/kg-day	subchronic	oral r	at Vaille et	PPRTV (
		+	8	NOEL	Renal	subchronic	5000.0	mg/kg-day	subchronic	oral r	at Vaille et	PPRTV (
		+	8	LOEL	Systemic	subchronic	2500.0	mg/kg-day	subchronic	oral r	at Vaille et	PPRTV (
		+	8	NOEL	Hematol	subchronic	1500.0	mg/kg-day	subchronic	oral ra	bbit Vaille et	PPRTV (
		+	8	NOEL	Systemic	subchronic	1500.0	mg/kg-day	subchronic	oral ra	bbit Vaille et	PPRTV (

In Vitro Bioassay Screening ToxCast and Tox21





13

Sources of Exposure to Chemicals



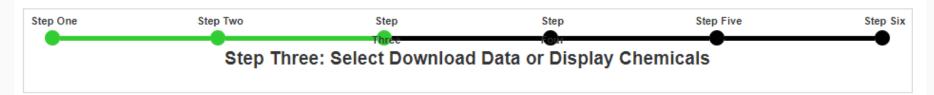
Product & Use Categories	osure	Bioassays	Similar Compounds	Related Substances	Synonyms	Literature	Links	Commen	ts
Chemical Weight Fraction		Proc	duct & Use Categorie	es (PUCs) 🚯					
Chemical Functional Use	_	Categorizat	<u>tion type</u>	\$ <u>Nu</u> 288	mber of Unique P	roducts		•	*
Monitoring Data		PUC PUC		208					
Exposure Predictions		PUC PUC		107	,				
		PUC		101					
Production Volume		PUC		90 89					-

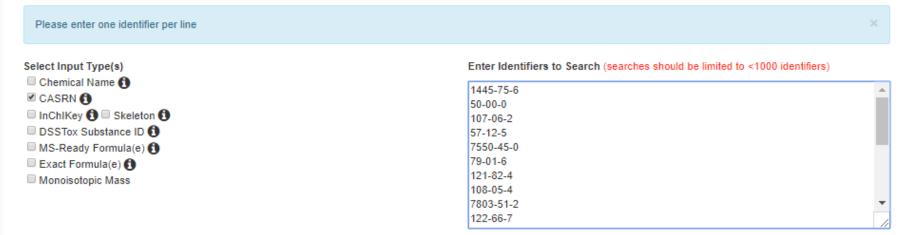
Batch Searches

2









Display All Chemicals Download Chemical Data

Batch Search



Intrinsic And Predicted Properties

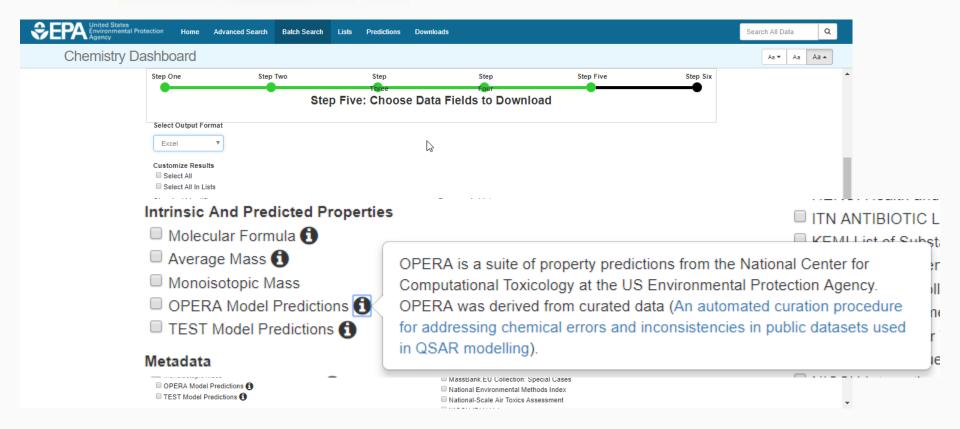
- 🗏 Molecular Formula 🚯
- Average Mass 1
- Monoisotopic Mass
- OPERA Model Predictions
- TEST Model Predictions 1

Metadata

- Curation Level Details (1)
- 🗆 Data Sources 🚯
- Assay Hit Count
- Include links to ACToR reports SLOW! (BETA) 1
- NHANES/Predicted Exposure 1
- Include ToxVal Data Availability (1)
- Number of PubMed Articles (1)
- Abstract Sifter Input File (Beta) (1)
- MetFrag Input File(Beta)
- IRIS
- PPRTV
- PubChem Data Sources

OPERA and TEST in Batch





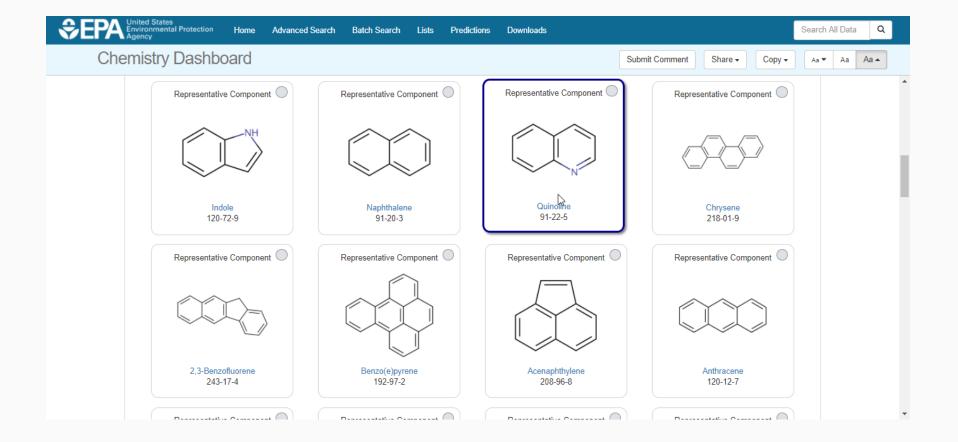
Excel Output



	А	В	С	D	E	F	G	Н
1	INPUT	FOUND_BY	DTXSID	PREFERRED_NAME	EXPOCAS	EXPOCAS	NHANES	TOXVAL_D
2	1445-75-6	CAS-RN	DTXSID5024051	Diisopropyl methylpho:	2.09e-08	Y	-	Y
3	50-00-0	CAS-RN	DTXSID7020637	Formaldehyde	1.32e-06	Y	-	Y
4	107-06-2	CAS-RN	DTXSID6020438	1,2-Dichloroethane	4.9e-06	Y	-	Y
5	57-12-5	CAS-RN	DTXSID6023991	Cyanide	-	-	-	Υ
6	7550-45-0	CAS-RN	DTXSID8042476	Titanium tetrachloride	-	-	-	Y
7	79-01-6	CAS-RN	DTXSID0021383	Trichloroethylene	7.27e-06	Y	-	Y
8	121-82-4	CAS-RN	DTXSID9024142	Cyclonite	6.72e-08	Y	-	Y
9	108-05-4	CAS-RN	DTXSID3021431	Vinyl acetate	8.3e-05	Y	-	Y
10	7803-51-2	CAS-RN	DTXSID2021157	Phosphine	-	-	-	Y
11	122-66-7	CAS-RN	DTXSID7020710	1,2-Diphenylhydrazine	1.49e-07	Y	-	Y
12	101-77-9	CAS-RN	DTXSID6022422	4,4'-Methylenedianiline	6.08e-06	Y	-	Y
13	14017-34-6	CAS-RN	DTXSID90161250	Selenium difluoride	-	-	-	-
14	75-44-5	CAS-RN	DTXSID0024260	Phosgene	-	-	-	Y
15	621-64-7	CAS-RN	DTXSID6021032	N-Nitrosodipropylamine	4.55e-07	Y	-	Y
16	75-09-2	CAS-RN	DTXSID0020868	Dichloromethane	2.02e-06	Y	-	Y
17	100-41-4	CAS-RN	DTXSID3020596	Ethylbenzene	8.32e-05	Y	-	Y
18	7440-28-0	CAS-RN	DTXSID2036035	Thallium	-	-	-	Y
19	108-88-3	CAS-RN	DTXSID7021360	Toluene	8.61e-05	Y	-	Y
20	111-44-4	CAS-RN	DTXSID9020168	Bis(2-chloroethyl) ethe	2.82e-07	Y	-	Y
21	7440-42-8	CAS-RN	DTXSID3023922	Boron	-	-	-	Y
22	7440-29-1	CAS-RN	DTXSID6049800	Thorium	-	-	-	Y

Families of chemicals Polyaromatic Hydrocarbons





Not all chemicals are "structures"

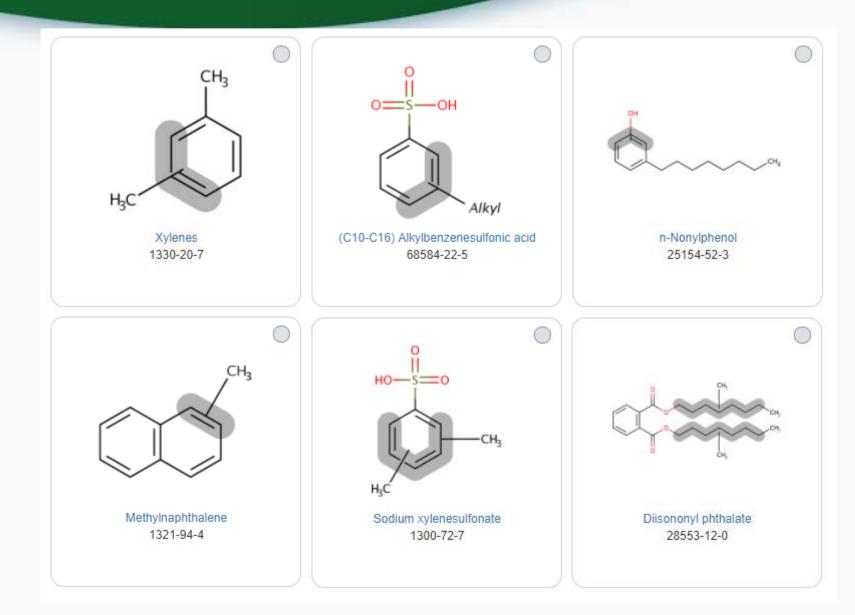


- UVCBs are chemical substances of unknown or variable composition, complex reaction products and biological materials
 - Surfactants (C11-14 linear alkyl sulfonates)
 - Reaction mass of p-t-butylphenyldiphenyl phosphate and bis(p-t-butylphenyl)phenyl phosphate and triphenyl phosphate
 - Almond Oil

"Markush Structures"

https://en.wikipedia.org/wiki/Markush_structure

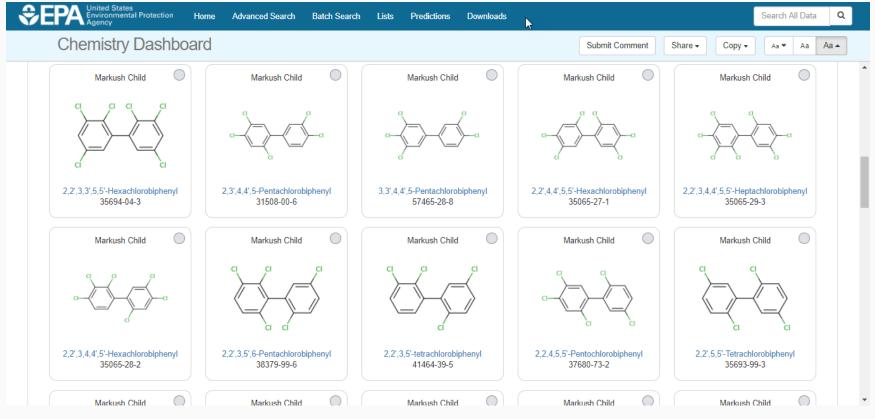




Enumeration of Markush



Markush structures can be enumerated into chemical families



From Dashboard to Prioritization



- Can we bring data together to prioritize risk?
 - Integrated dashboard data can be used to rank order and prioritize risk
- Internal application in development to use scoring to prioritize risk – uses combination of available experimental data and new assessment methods (NAMs)

Potential Data Sources



In Vivo Human Hazard:

- Mammalian toxicity studies guideline-like, use POD
- System-specific *in vivo* data (Cancer, developmental)
- Models (QSAR) to predict POD and organ-specific effects
- Genotoxicity
- In vitro-derived endocrine disruption and neurotoxicity models

In Vivo Eco Hazard

- Aquatic in vivo studies POD
- Models (QSAR) of POD

Potential Data Sources



Human Exposure

- Data on production volume and releases
- Quantitative biomonitoring data
- Predictions of oral and inhalation exposure

Eco Exposure

- Biomonitoring data
- Predictions of water concentrations

Physchem

• Persistence and Bioaccumulation models (OPERA)

Mansouri et al. J Cheminform (2018) 10:10 https://doi.org/10.1186/s13321-018-0263-1 Journal of Cheminformatics



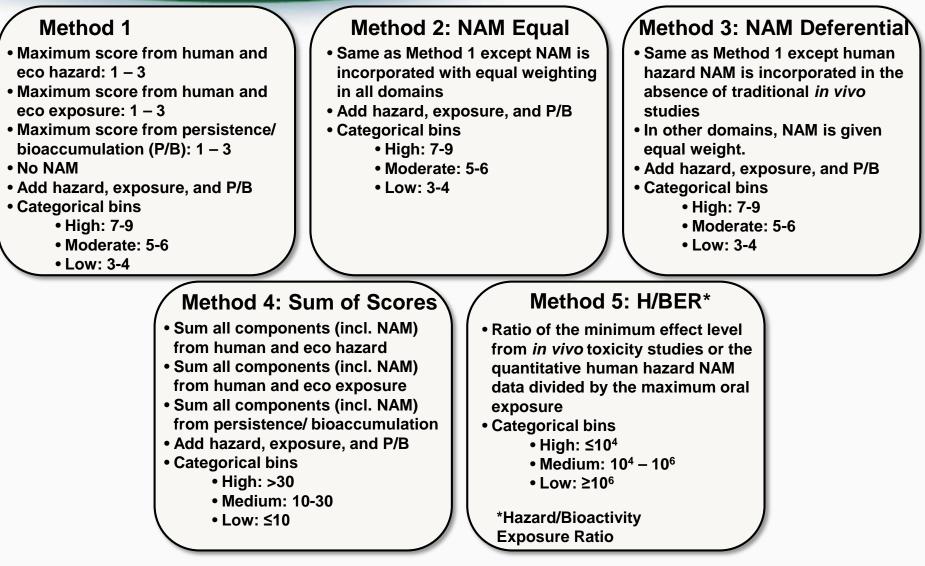
Scoring approaches



- For each chemical, each domain receives a score of 1 (Low), 2 (Moderate), or 3 (High) concern
- Hazard score = maximum of human and eco hazard scores
- **Exposure score** = maximum of human and eco exposure scores
- **Total score** = hazard score + exposure score + physchem score
- If no data is available for a domain, it is given the "missing data score", currently 1 (Low)
- Scoring can include or exclude NAM

Implemented Scoring Methods





Overall Scoring Page



Phy	schem	Pri	oritization	
Show	25	~	entries	

Domain Help

Cutoffs

Human Hazard Prioritization

Eco Hazard Prioritization

Human Exposure Prioritization

Eco Exposure Prioritization

Overall Prioritization

Data Coverage Summary Distribution Graphs

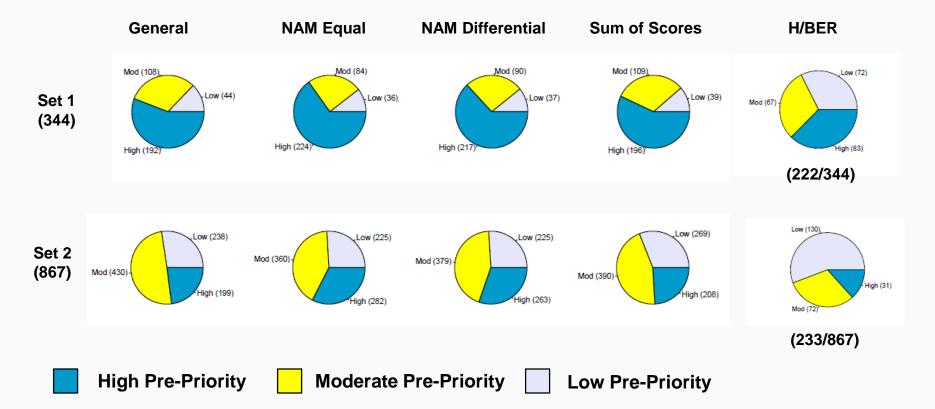
on Graphs

Search:

DSSTox_ID	CASRN	Name	[−] ♦ Method [♦] 1 score	Method 1 bin	Method 2 score	Method 2 bin	Method 3 score	Method 3 bin	♦ Method 4 score	¢ Method 4 bin
DTXSID124356	1234-56-7	Name1	5	Moderate (ExeHzeHzh)	6	Moderate (ExeHzeHzh)	6	Moderate (ExeHzeHzh)	25	Moderate (ExeHzeHzh)
DTXSID124357	1234-56-8	Name2	5	Moderate (PbExeHzeHzh)	7	High (PbExeHzeHzh)	7	High (PbExeHzeHzh)	24	Moderate (PbExeHzeHzh)
DTXSID124358	1234-56-9	Name3	I- 5	Moderate (ExeHzeHzh)	6	Moderate (ExeHzeHzh)	6	Moderate (ExeHzeHzh)	41	High (ExeHzeHzh)
DTXSID124359	1234-56-10	Name4	5	Moderate (ExeHzeHzh)	5	Moderate (ExeHzeHzh)	5	Moderate (ExeHzeHzh)	13	Moderate (ExeHzeHzh)
DTXSID124360	1234-56-11	Name5	5	Moderate (PbExeHzeHzh)	5	Moderate (PbExeHzeHzh)	5	Moderate (PbExeHzeHzh)	20	Moderate (PbExeHzeHzh)
DTXSID124361	1234-56-12	Name6	5	Moderate (ExeHzeHzh)	5	Moderate (ExeHzeHzh)	5	Moderate (ExeHzeHzh)	35	High (ExeHzeHzh)
DTXSID124362	1234-56-13	Name7	5	Moderate (PbExeHze)	5	Moderate (PbExeHze)	5	Moderate (PbExeHze)	21	Moderate (PbExeHze)
DTXSID124363	1234-56-14	Name8	6	Moderate (PbExeHze)	6	Moderate (PbExeHze)	6	Moderate (PbExeHze)	16	Moderate (PbExeHze)
DTXSID124364	1234-56-15	Name9	5	Moderate (PbExeHze)	5	Moderate (PbExeHze)	5	Moderate (PbExeHze)	26	Moderate (PbExeHze)
DTXSID124365	1234-56-16	Name10	6	Moderate (PbExeHze)	6	Moderate (PbExeHze)	6	Moderate (PbExeHze)	23	Moderate (PbExeHze)
DTXSID124366	1234-56-17	Name11	5	Moderate	5	Moderate	5	Moderate	17	Moderate >

Fraction of chemicals in each bin



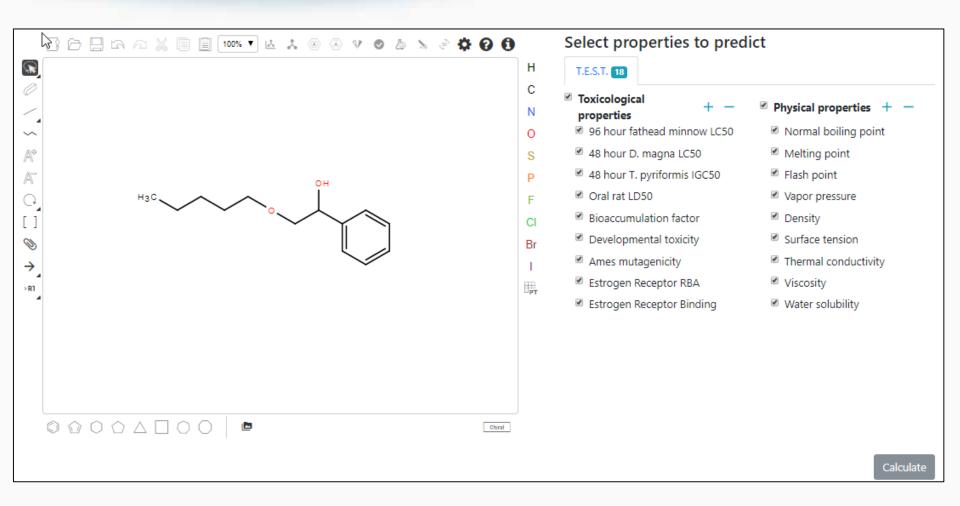




- Present work in development
 - Real time OPERA predictions TEST predictions done

Real-Time Predictions





Real-Time Predictions

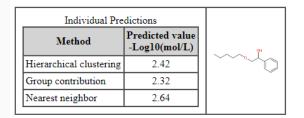


		Experimental			Prediction		
	Property	Value	Consensus	Hierarchical clustering	Single model	Group contribution	Nearest neighbor
6	96 hour fathead minnow LC50		4.477 -Log10(mol/L) 6.954 mg/L	4.195 -Log10(mol/L) 13.288 mg/L	3.994 -Log10(mol/L) 21.110 mg/L	3.478 -Log10(mol/L) 69.224 mg/L	6.238 -Log10(mol/L) 0.120 mg/L
	48 hour D. magna LC50		4.398 -Log10(mol/L) 8.328 mg/L	3.877 -Log10(mol/L) 27.677 mg/L	4.039 -Log10(mol/L) 19.026 mg/L	4.084 -Log10(mol/L) 17.173 mg/L	5.593 -Log10(mol/L) 0.532 mg/L
	48 hour T. pyriformis IGC50		4.063 -Log10(mol/L) 18.039 mg/L	3.731 -Log10(mol/L) 38.668 mg/L		3.386 -Log10(mol/L) 85.610 mg/L	5.070 -Log10(mol/L) 1.773 mg/L
	Oral rat LD50		1.758 -Log10(mol/kg) 3640.950 mg/kg	1.982 -Log10(mol/kg) 2172.756 mg/kg			1.533 -Log10(mol/kg) 6101.245 mg/kg
	Bioaccumulation factor		1.797 Log10 62.700	2.202 Log10 159.310	1.287 Log10 19.346	1.181 Log10 15.157	2.520 Log10 330.834
	Developmental toxicity		false	false	false		true
	Ames mutagenicity		false	false			false
	Estrogen Receptor RBA		-3.075 Log10 8.418*10 ⁻⁴	-3.078 Log10 8.356*10 ⁻⁴	-3.720 Log10 1.907*10 ⁻⁴		-2.427 Log10 0.004
	Estrogen Receptor Binding		true	true	true	false	true

Real-Time Predictions

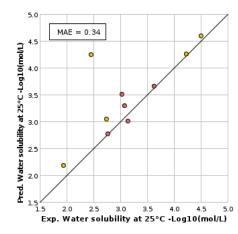
Predicted Water solubility at 25°C for OC(C=1C=CC=CC1)COCCCCC from Consensus method

Prediction results								
Endpoint	Experimental value	Predicted value						
Water solubility at 25°C -Log10(mol/L)	N/A	2.46						
Water solubility at 25°C mg/L	N/A	723.26						



Predictions for the test chemical and for the most similar chemicals

Rediction results (colors defined in table below)



Chemicals	MAE*				
Entire set	0.58				
Similarity coefficient ≥ 0.5	0.34				
*Mean absolute error in -Log10(mol/L)					

CAS	Structure	Similarity Coefficient	Experimental value -Log10(mol/L)	Predicted value -Log10(mol/L)
OC(C=1C=CC=CC1)COCCCCC (test chemical)			N/A	2.46
<u>104-40-5</u>	Û	0.68	4.50	4.60
<u>1219-38-1</u>		0.67	4.22	4.26





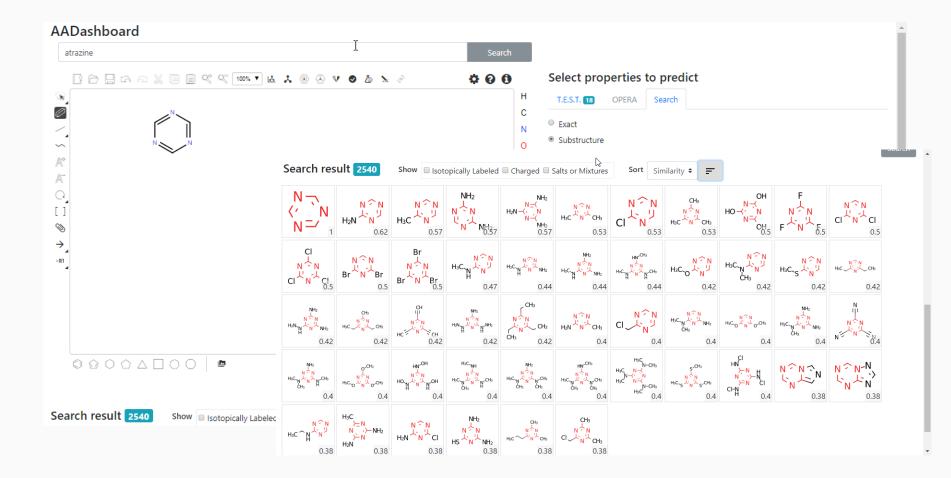


• Present work in development

- Real time OPERA prediction
- Structure/substructure/similarity search

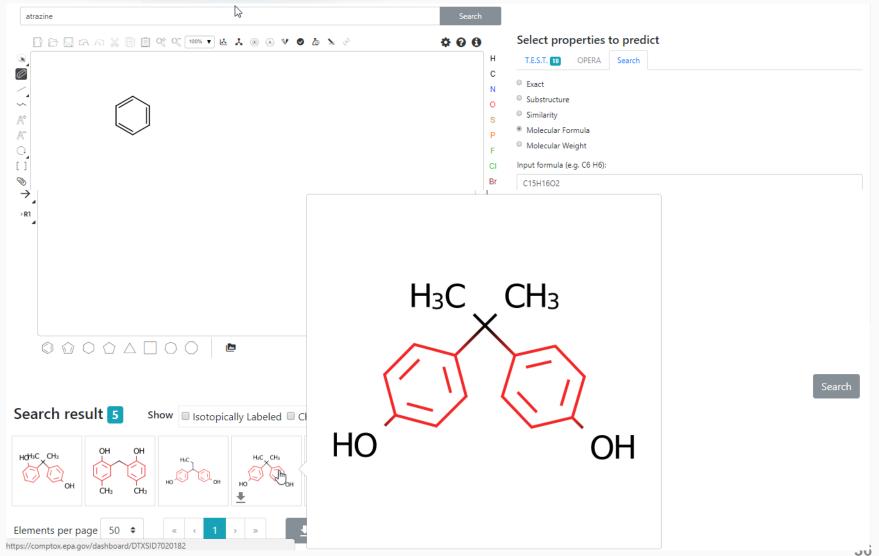
Prototype Development





Prototype Development





Work in Progress

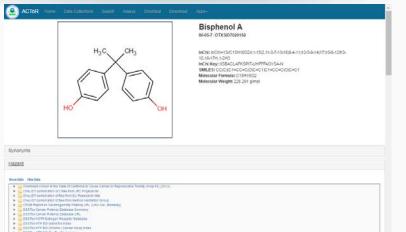


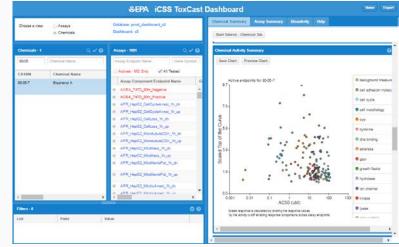
• Present work in development

- Real time OPERA prediction
- Structure/substructure/similarity search
- Merging in other NCCT dashboard capabilities

Earlier Dashboard Applications

United States Environmental Protection Agency





EPA United States	Indiana dal Protec	1914-1919			
Cat: Chemical and a are here: EPA.Homa - C		gories cology Research - Chemica	i Use		El Contact Us
D)tome D Search	* Results	a Dictionary & Downlo	and Alterp		
Chemical: BISPHENCL					
	CA	SRN: 80-05-7			
Export Use Data	CH Export Produ				
CPCat Descrip	stion o	Source Description o	ACTOR Data SetUat ::	Source ¢	Class of Chemical Category :
consumer_use_ACToRUseDB		Consumer Use		ACTOR UseDB	Use Categories
personal_care_ACToRUseDB		Personal Care Product		ACToR UseDB	Use Categories
industrial_manufacturing_ACToRUseD8		Chemical Industrial		ACTOR UseDB	Use Categories
child_use detected		Consumer Products	The Daniah EPA Exposure of 2-year-olds to chemical substances in Comsumer Products. This project included a survey of the products as well as chemical analyses and risk assessments of a number of selected products that 2 year-old thidlen to now into context with	ACToR Data Sets and Lists	Use Categories

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	United States Environmental Protection Agency	EDSP21 Dashboard Endocrine Diaruption Screening Program for the 21st Century
benical Surmary	Public Information Disardivity Sur	many Binachity High-Throughout Exposure Array Deficitions Terminativ
CDSP Dashboard Over	-	
EDSP Dashboard 0	Overview	
Congress requires EPA Screening Program for s	Endocrine Disructor Screening Program the 21st Century Dashboard (EDSP2) Dashboard (EDSP2) Dashboard (EDSP2)	to evaluate chemicals for potential endocrine disruption, and there are thousands of interest to the program. EPA researchers developed the Endocrine Disruption integrati to provide access to new chemical data on over 1,000 chemicals of interest.
The purpose of the EDS	IP21 Dashboard is to help the Endoonne D	Isruptor Screening Program evaluate chemicals for endocrine-related activity.
The data for this version	of the Dashboard comes from various so	ries :
 Chenical exposit High quality shere 	d (or in vitro high-throughput) shemical som re data and prediction models (Exps/CastE nical structures and annotations (DSSToc) arties Database (Phys/Chen/DB).	
ToxCast Data Use C	Considerations	
Careful review is	required to determine the use of the data is	essarily mean that it will assue taxing or an adverse health subcome. There are many factors that determine whether a chemical will assue a specific adverse health subcome. n a particular devices correct. me as contribut assure and malycical methods improve.
EPA will continuously as	of functionality and improve overall usabilit	y and performance.
To get the best possible	experience using the EDSP Dashboard ay	oplication we recommend using Mozilla Fireflex or Google Chrome.
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Work in Progress



• Present work in development

- Real time OPERA prediction
- Structure/substructure/similarity search
- Merging in other NCCT dashboard capabilities
- Web-services for community consumption
 - TEST predictions already available
 - Chemical Resolver service
 - Embeddable widgets

Conclusion



- The CompTox Chemistry Dashboard provides access to data for ~760,000 chemicals
- Multiple prediction models available for data gap filling
 - OPERA models and TEST models PhysChem and Tox endpoints
 - Models based on *in vitro* data classification models
 - Generalized Read-Across development in progress
- Real time prediction models rollout has started
- Web services available for some physchem and toxicity endpoints
- 2 years development as a CompTox Integration Hub





Antony Williams

US EPA Office of Research and Development

National Center for Computational Toxicology (NCCT)

Williams.Antony@epa.gov

ORCID: https://orcid.org/0000-0002-2668-4821