

The EPA Comptox Chemistry Dashboard: A Web-Based Data Integration Hub

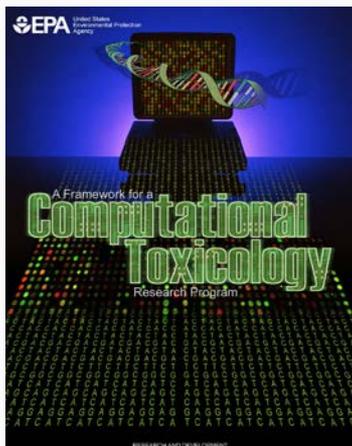
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U.S. Environmental Protection Agency, RTP, NC

This work was reviewed by the U.S. EPA and approved for presentation but does not necessarily reflect official Agency policy.

*Luxembourg Centre for Systems Biomedicine
27th November 2017*

National Center for Computational Toxicology

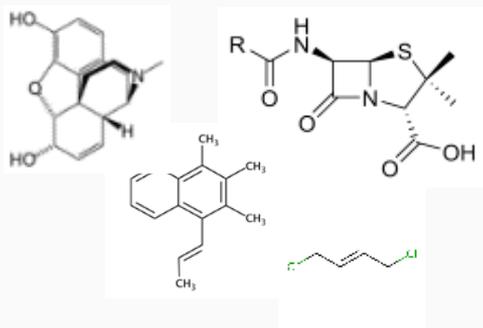


- National Center for Computational Toxicology established in 2005 to integrate:
 - High-throughput and high-content technologies
 - Modern molecular biology
 - Data mining and statistical modeling
 - Computational biology and chemistry
- Staffed by ~60 employees and contractors as part of EPA's Office of R&D
- Home of ToxCast & ExpoCast research efforts
- Key partner in U.S. Tox21 federal consortium
- Multiple cross-division collaborations (e.g. NERL, OPP, OPPT)

- Our team is broad in skills
 - Biologists, chemists and toxicologists
 - Bioinformaticians and cheminformaticians - modelers (QSAR, Deep Learning), text miners
 - Information technology team, software developers
 - A large IT support team for production applications (National Computing Center)

Why we must innovate...

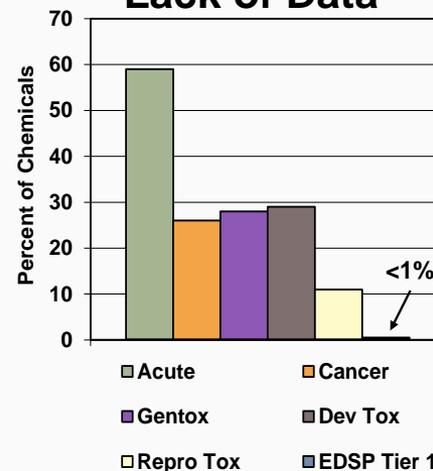
Number of Chemicals /Combinations



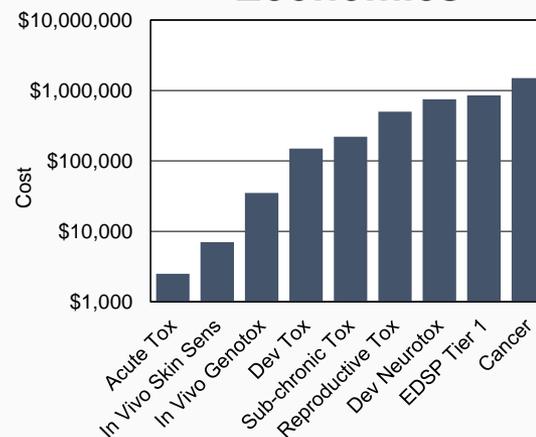
Ethical Concerns



Lack of Data



Economics



TSCA Chemical Substance Inventory

- Inventory was initially published in 1979
- Second version, containing about 62k chemical substances, was published in 1982
- Continues to grow and now lists ~85k chemicals, about 15k are confidential business information

The need for data and derivative models and algorithms

- NCCT outputs: include a lot of data, models, algorithms and software applications
- We produce Open Data – we want people to interrogate it, learn from it, develop understanding

Toxicity Forecasting

Advancing the Next Generation of Chemical Evaluation

EPA needs rapid and efficient methods to prioritize, screen and evaluate thousands of chemicals. EPA's Toxicity Forecaster (ToxCast) generates data and predictive models on thousands of chemicals of interest to the EPA. ToxCast uses high-throughput screening methods and computational toxicology approaches to rank and prioritize chemicals. In fact, EPA's Endocrine Disruption Screening Program (EDSP) is working to use ToxCast to rank and prioritize chemicals.



- ToxCast has data on over 1,800 chemicals from a broad range of sources including industrial and consumer products, food additives, and potentially "green" chemicals that could be safer alternatives to existing chemicals.
- ToxCast screens chemicals in over 700 high-throughput assays that cover a range of high-

Downloadable Computational Toxicology Data

EPA's computational toxicology research efforts evaluate the potential health effects of thousands of chemicals. The process of evaluating potential health effects involves generating data that investigates the potential harm, or hazard of a chemical, the degree of exposure to chemicals as well as the unique chemical characteristics.

As part of EPA's commitment to share data, all of the computational toxicology data is publicly available for anyone to access and use.

High-throughput Screening Data

EPA researchers use rapid chemical screening (called high-throughput screening assays) to limit the number of laboratory animal tests while quickly and efficiently testing thousands of chemicals for potential health effects.

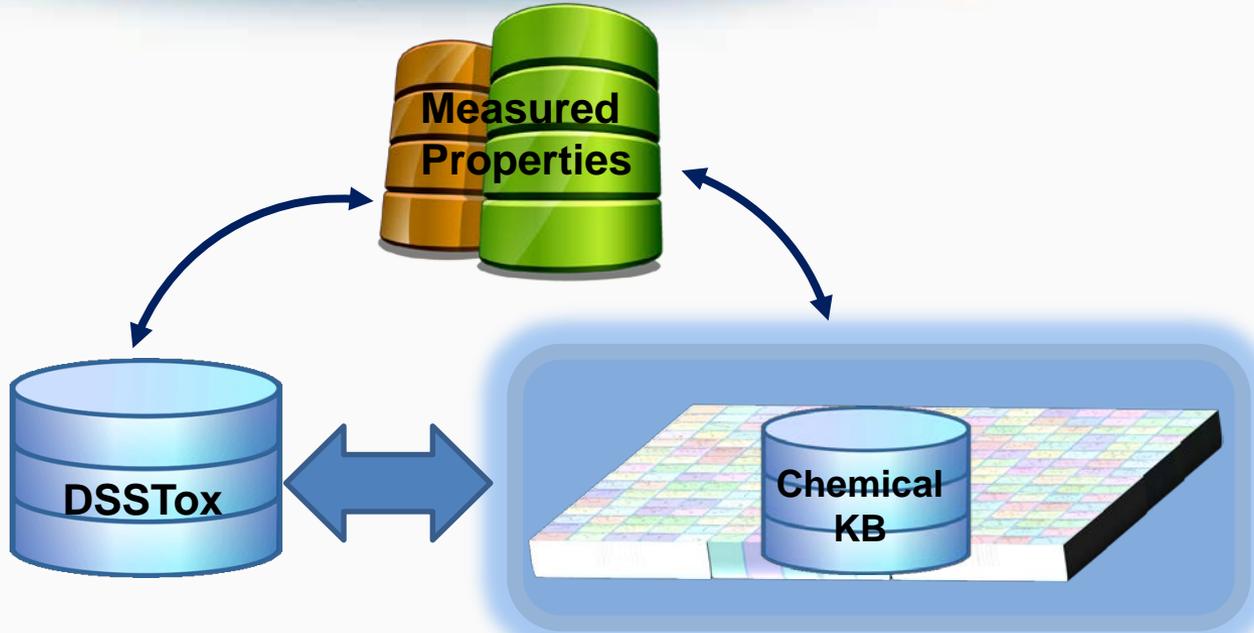
- [ToxCast Data](#): High-throughput screening data on thousands of chemicals.

Rapid Exposure and Dose Data

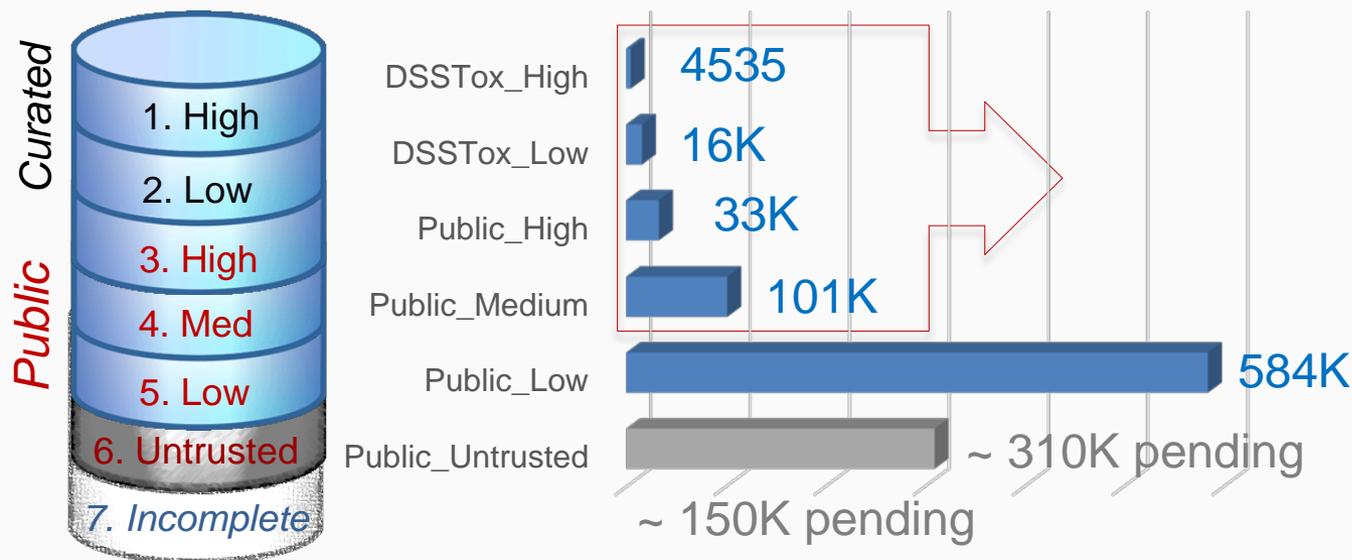
EPA researchers develop and use rapid exposure estimates to predict potential exposure for thousands of chemicals.

- [High-throughput toxicokinetics data](#): It is important to link the external dose of a chemical to an internal blood or tissue concentration. This process is called toxicokinetics. EPA researchers measure the critical factors that determine the distribution

Underpinning with chemicals



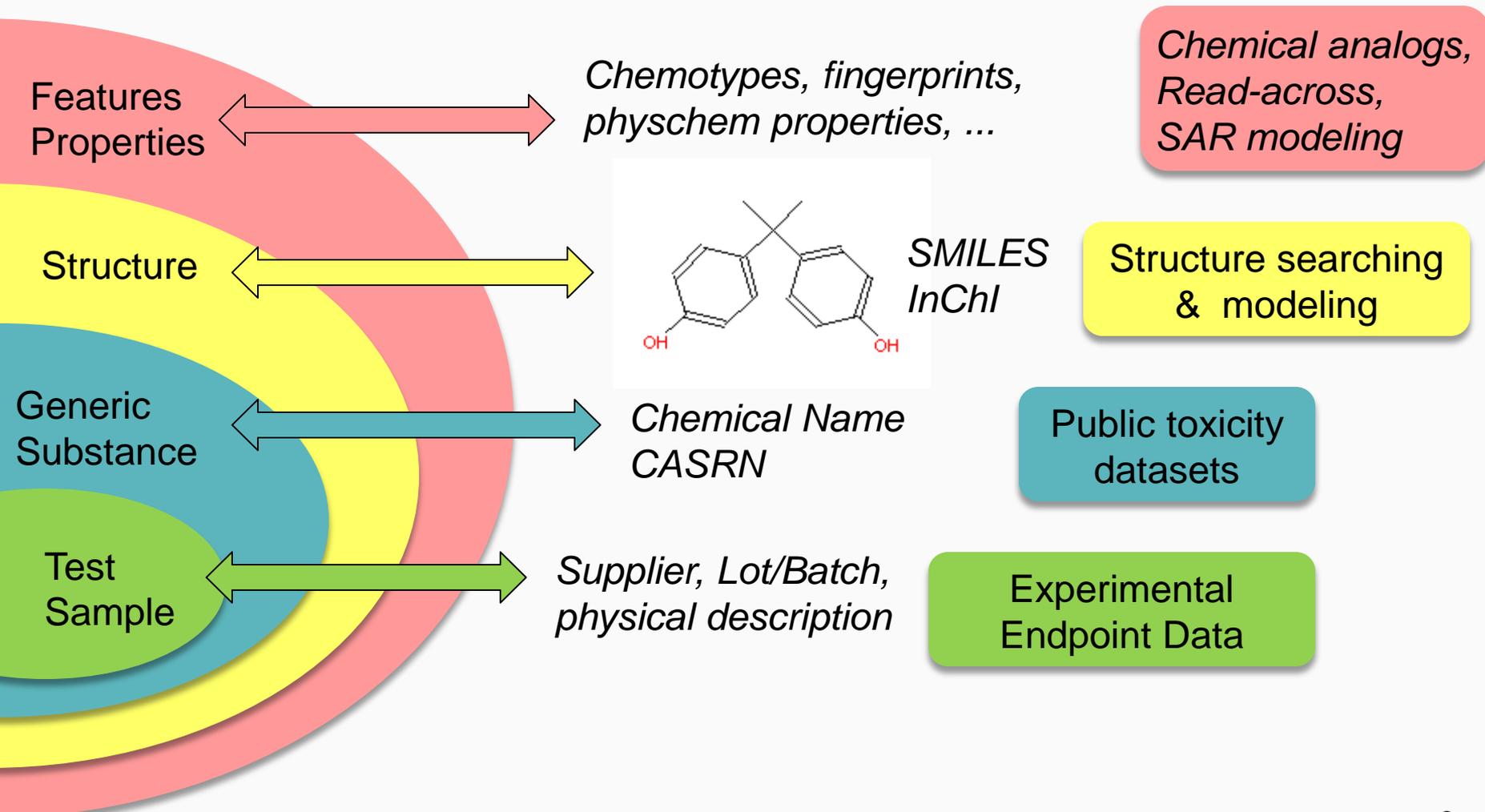
Approximately 17 Years of Data... Growing with daily curation



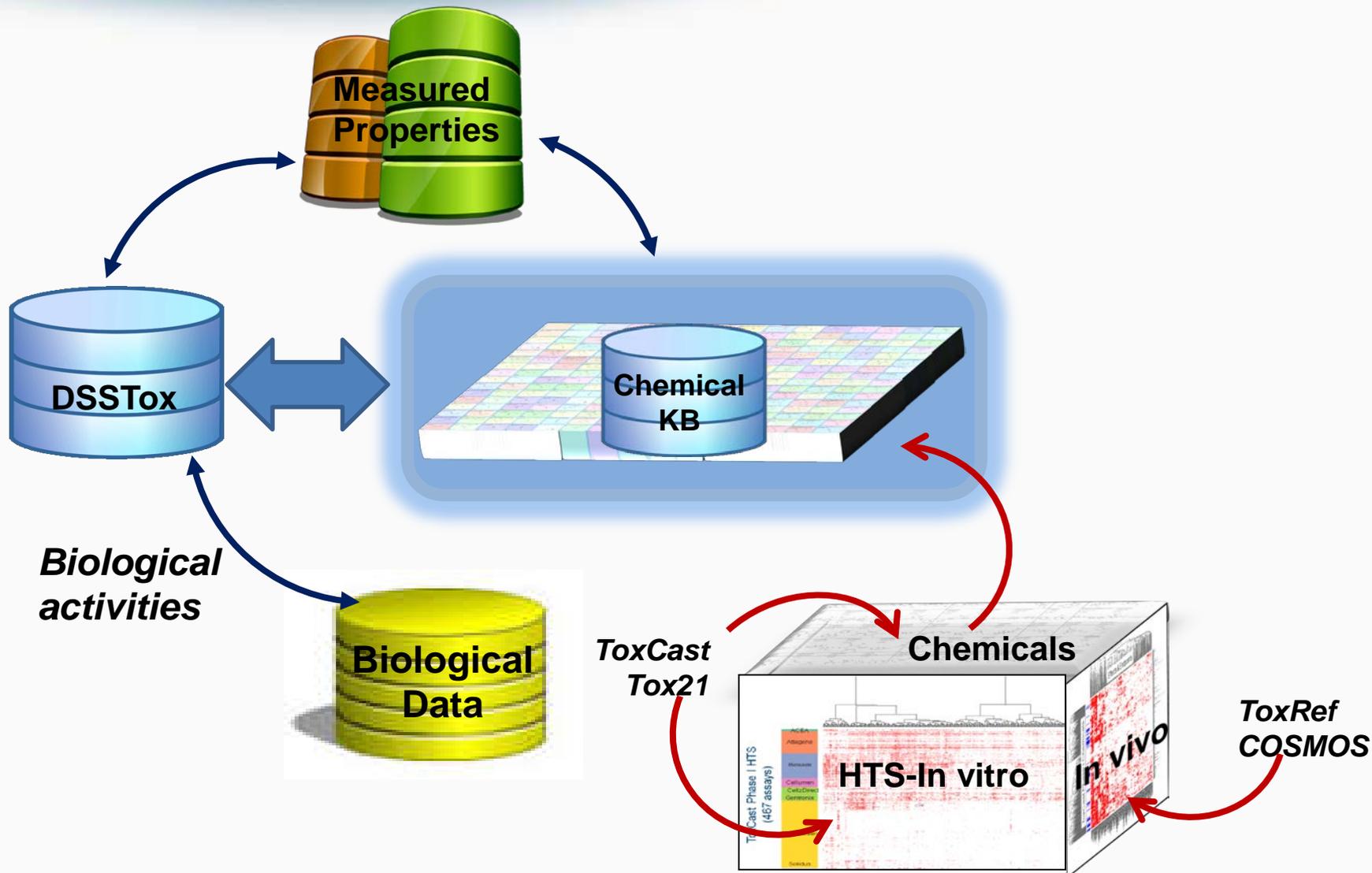
QC Levels

DSSTox_High:	Hand curated and validated
DSSTox_Low:	Hand curated and confirmed using multiple public sources
Public_High:	Extracted from EPA SRS and confirmed to have no conflicts in ChemID and PubChem
Public_Medium:	Extracted from ChemID and confirmed to have no conflicts in PubChem
Public_Low:	Extracted from ACToR or PubChem
Public_Untrusted:	Postulated, but found to have conflicts in public sources

Chemical representation levels supporting data integration

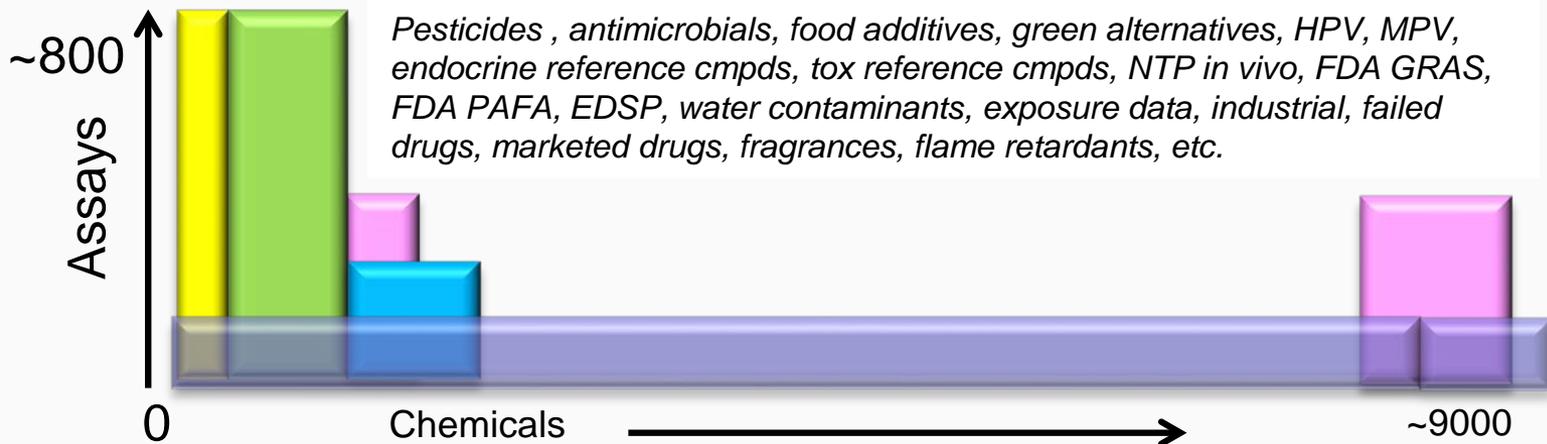


Integrating *in vitro* and *in vivo* data

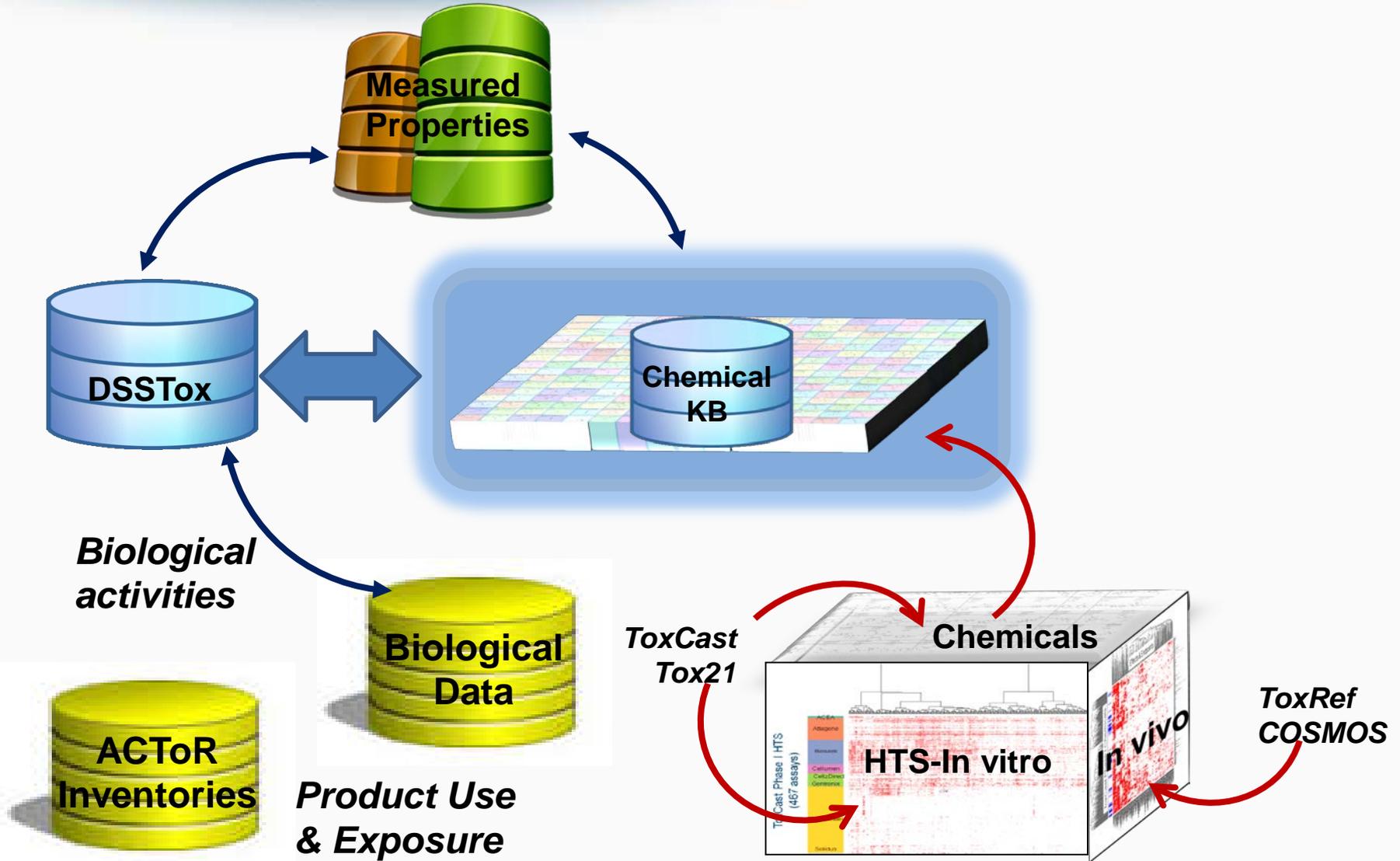


TEN YEARS of Assay Measurements: ToxCast & Tox21

Set	Chemicals	Assays	Endpoints	Completion
ToxCast Phase I	293	~600	~700	2011
ToxCast Phase II	767	~600	~700	03/2013
ToxCast E1K	800	~50	~120	03/2013
ToxCast Phase III	~900	~300	~300	In progress
Tox21	~9000	~80	~150	In progress



Adding Product Use and Exposure



High Throughput Measurement to Identify Exposure



Rapid Chemical Exposure and Dose Research

EPA is responsible for ensuring the safety of thousands of chemicals. Quantitative exposure data are available for only a small fraction of registered chemicals. This type of exposure data is needed to thoroughly evaluate chemicals for potential risks to humans, wildlife and ecosystems. EPA is developing innovative methods to develop exposure estimates for thousands of chemicals to better protect human health and the environment. These innovative methods are called rapid exposure and dose assessments.

Rapid Exposure Predictions

Rapid, also called high-throughput, exposure predictions or ExpoCast provide rapid exposure estimates for thousands of chemicals. ExpoCast quickly and efficiently looks at multiple routes of exposure to provide exposure estimates. ExpoCast uses and enhances two well-known exposure models to estimate chemical exposure.

- [Farfield Exposure Models](#)
- [Nearfield Exposure Models](#)

Evaluating High-throughput Exposure Predictions

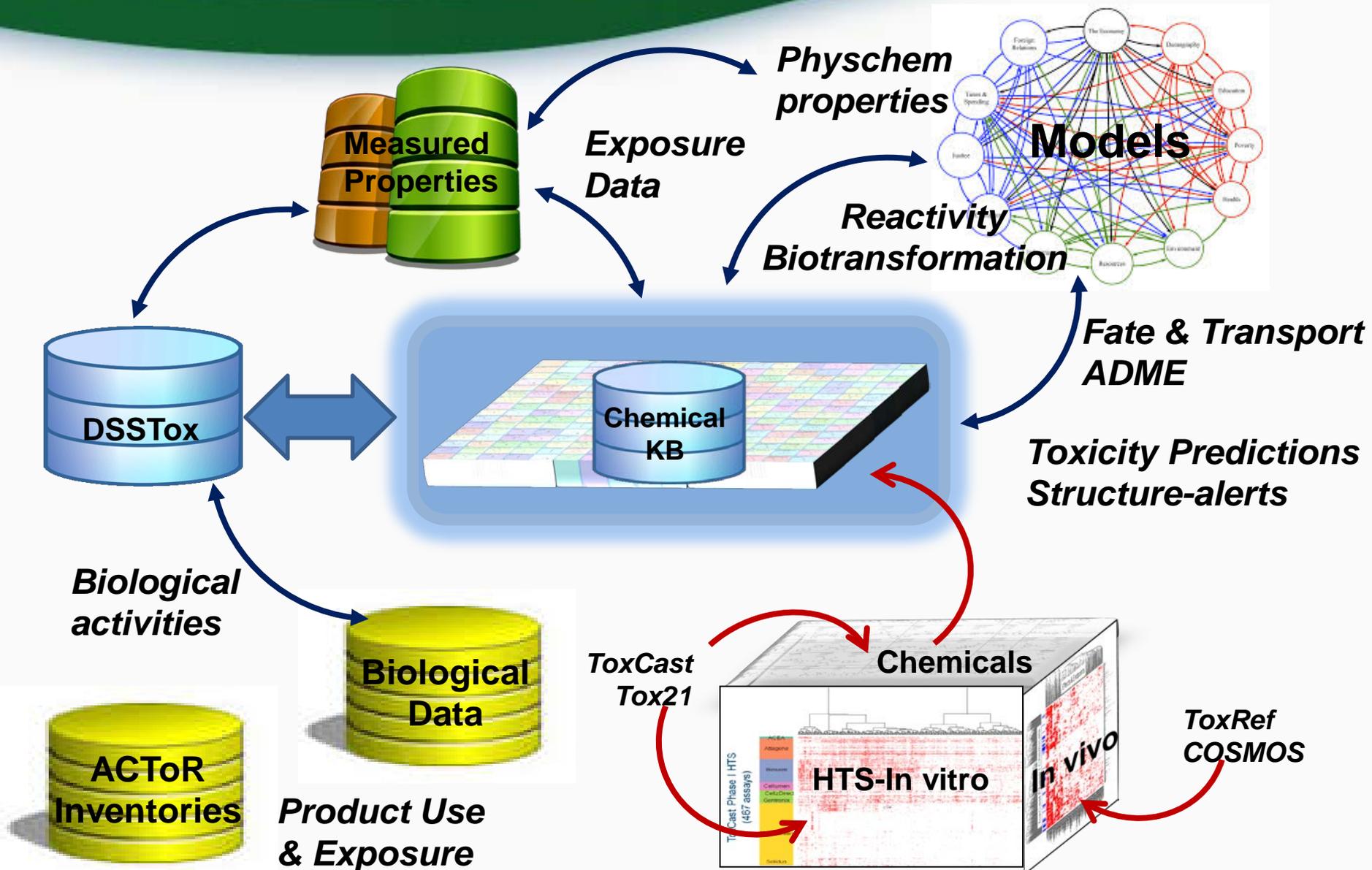
EPA is currently evaluating the effectiveness of high-throughput exposure models



Pictured Above: Farfield Exposure Examples



Building Models from the data



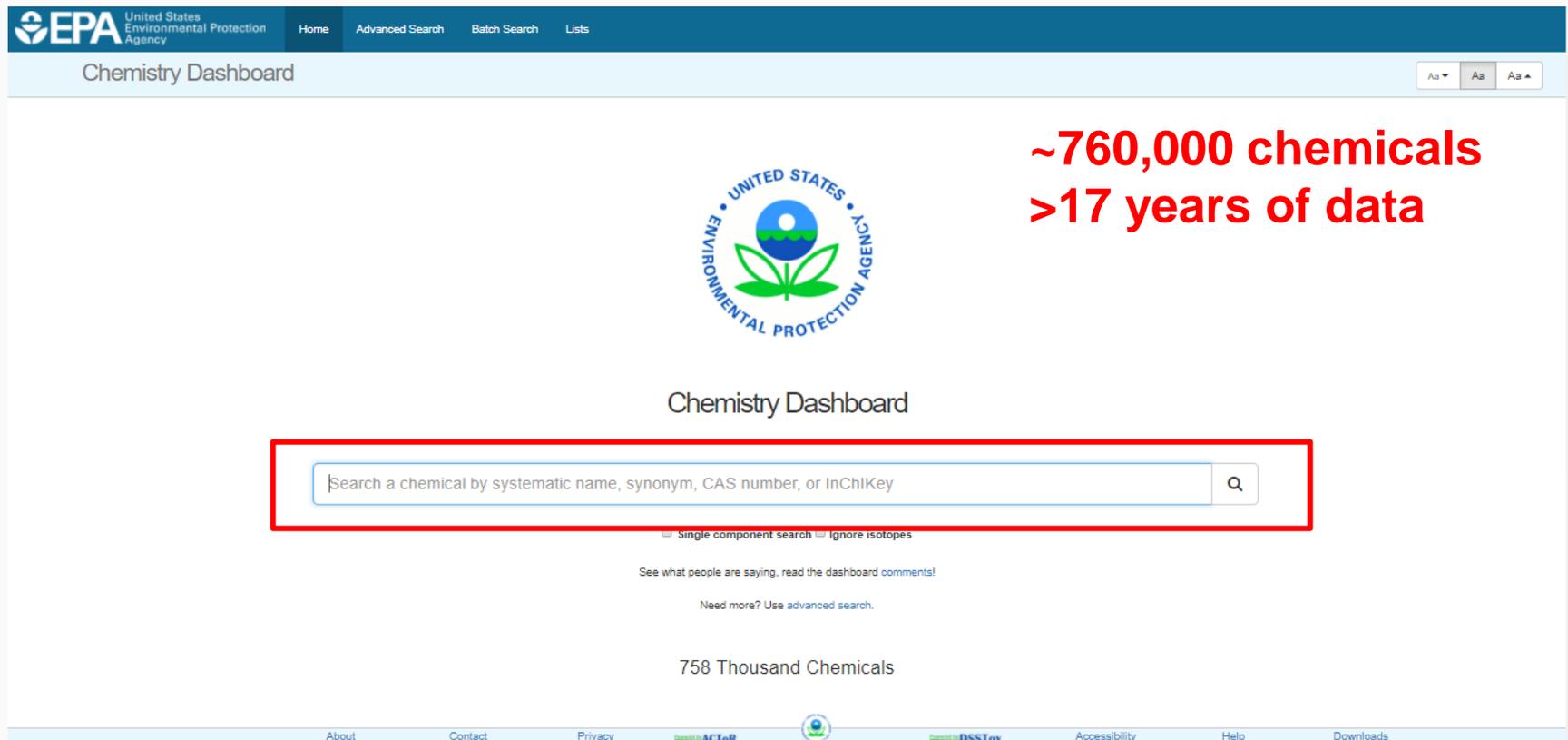
- Data curation, standardization and versioning is **essential**
- **Prototype** application development suffices for **research** projects
- **Production apps** need managed processes
- ODOSOS (Open Data, Open Source and Open Standards) endows many benefits

The CompTox Chemistry Dashboard: An Overview

- **A publicly accessible website** delivering access:
 - ~760,000 chemicals and related property data
 - Links to other agency websites and public data resources
 - “Literature” searches for chemicals using public resources
 - Integration to “biological assay data” for 1000s of chemicals
 - Information regarding consumer products containing chemicals
 - “Batch searching” for thousands of chemicals
- Day-to-day curation efforts for data quality

Comptox Chemistry Dashboard

<https://comptox.epa.gov>



United States Environmental Protection Agency

Home Advanced Search Batch Search Lists

Chemistry Dashboard

~760,000 chemicals
>17 years of data



Chemistry Dashboard

Search a chemical by systematic name, synonym, CAS number, or InChIKey

Single component search Ignore isotopes

See what people are saying, read the dashboard comments!

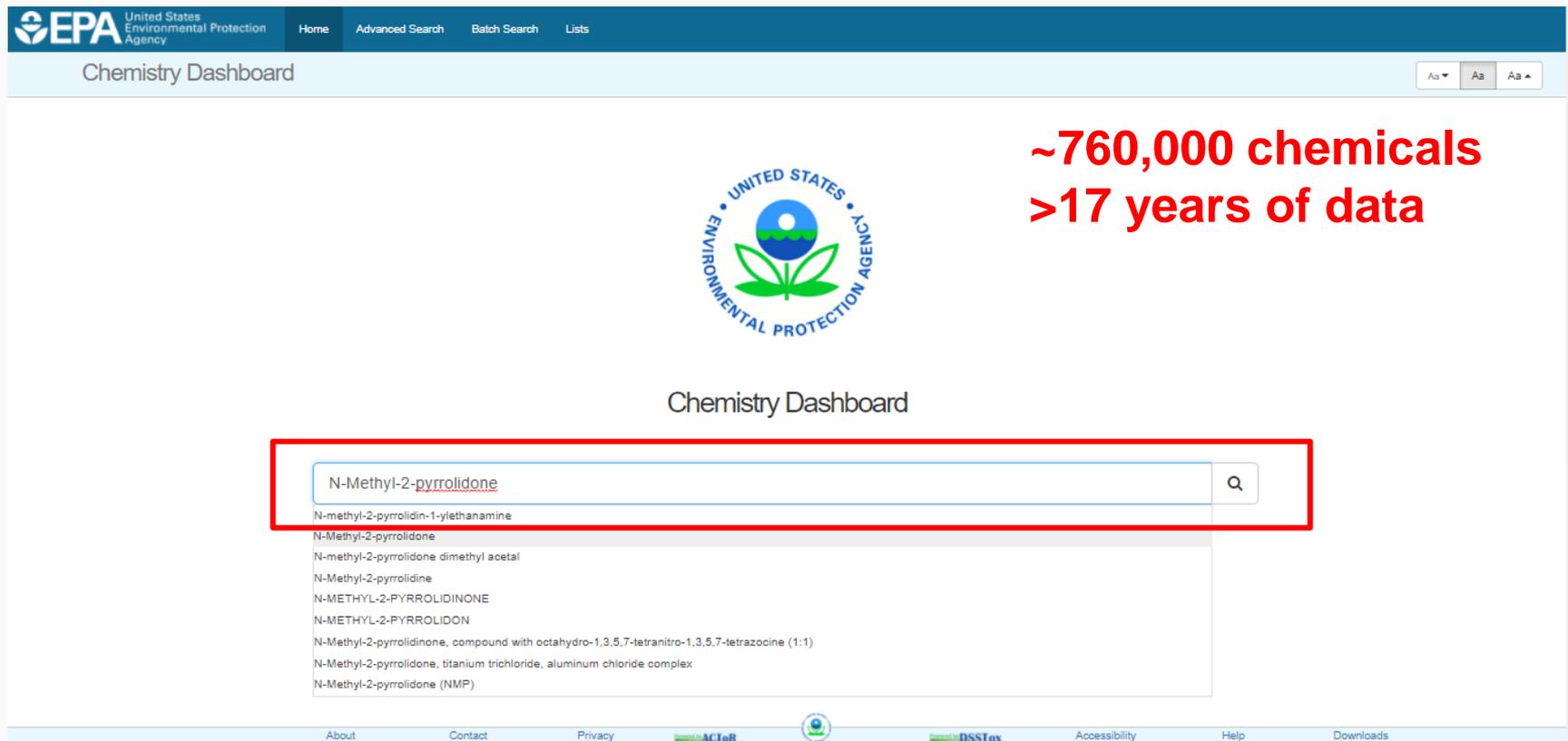
Need more? Use advanced search.

758 Thousand Chemicals

About Contact Privacy ACToR DSSTox Accessibility Help Downloads

Comptox Chemistry Dashboard

<https://comptox.epa.gov>



The screenshot shows the EPA Comptox Chemistry Dashboard interface. At the top, there is a navigation bar with the EPA logo and links for Home, Advanced Search, Batch Search, and Lists. Below this is a header for the Chemistry Dashboard with a search icon. The main content area features the EPA logo and the text "Chemistry Dashboard". A search bar is highlighted with a red box, containing the text "N-Methyl-2-pyrrolidone". Below the search bar, a list of search results is displayed, including "N-methyl-2-pyrrolidin-1-ylethanamine", "N-Methyl-2-pyrrolidone", "N-methyl-2-pyrrolidone dimethyl acetal", "N-Methyl-2-pyrrolidine", "N-METHYL-2-PYRROLIDINONE", "N-METHYL-2-PYRROLIDON", "N-Methyl-2-pyrrolidinone, compound with octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (1:1)", "N-Methyl-2-pyrrolidone, titanium trichloride, aluminum chloride complex", and "N-Methyl-2-pyrrolidone (NMP)". The footer contains links for About, Contact, Privacy, ACToR, DSSTox, Accessibility, Help, and Downloads.

United States
Environmental Protection
Agency

Home Advanced Search Batch Search Lists

Chemistry Dashboard

~760,000 chemicals
>17 years of data

Chemistry Dashboard

N-Methyl-2-pyrrolidone

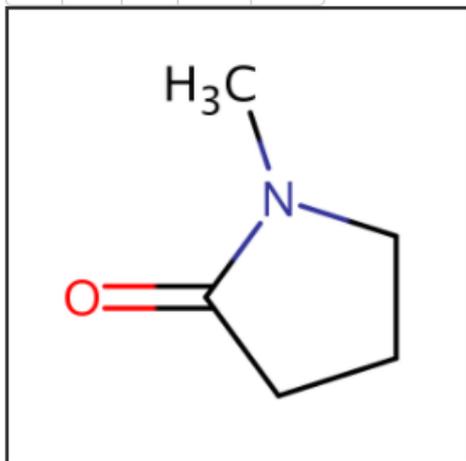
- N-methyl-2-pyrrolidin-1-ylethanamine
- N-Methyl-2-pyrrolidone
- N-methyl-2-pyrrolidone dimethyl acetal
- N-Methyl-2-pyrrolidine
- N-METHYL-2-PYRROLIDINONE
- N-METHYL-2-PYRROLIDON
- N-Methyl-2-pyrrolidinone, compound with octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (1:1)
- N-Methyl-2-pyrrolidone, titanium trichloride, aluminum chloride complex
- N-Methyl-2-pyrrolidone (NMP)

About Contact Privacy ACToR DSSTox Accessibility Help Downloads

N-Methyl-2-pyrrolidone

872-50-4 | DTXSID6020856

© Searched by Synonym from Valid Source: Found 1 result for 'N-METHYLPYRROLIDONE'.



Wikipedia

Intrinsic Properties

Molecular Formula: C₅H₉NO

Q Find All Chemicals 

Average Mass: 99.133 g/mol



Monoisotopic Mass: 99.068414 g/mol



Structural Identifiers

Related Compounds

Presence in Lists

Record Information

Chemical Properties

Env. Fate/Transport

Toxicity Values (Beta)

ADME (Beta)

Exposure

Bioassays

Similar Molecules (Beta)

Synonyms

Literature

External Links

Chemical Properties

Summary

Download as:

TSV

Excel

SDF

LogP: Octanol-Water

Water Solubility

Density

Flash Point

Melting Point

Boiling Point

Surface Tension

Thermal Conductivity

Vapor Pressure

Viscosity

LogKoa: Octanol-Air

Property	Average		Median		Range		Unit
	Experimental	Predicted	Experimental	Predicted	Experimental	Predicted	
LogP: Octanol-Water	-0.380 (1)	-0.329 (5)	-0.380	-0.329	-0.380	-0.494 to -0.110	-
Water Solubility	10.1 (1)	6.68 (4)	10.1	6.68	10.1	1.48 to 12.8	mol/L
Density	-	1.02 (2)	-	1.02	-	1.01 to 1.03	g/cm ³
Flash Point	-	75.7 (2)	-	75.7	-	65.2 to 86.1	°C
Melting Point	-23.8 (8)	1.32e-01 (4)	-24.0	1.32e-01	-24.0 to -23.0	-10.2 to 25.9	°C
Boiling Point	203 (6)	199 (5)	204	199	202 to 204	191 to 202	°C
Surface Tension	-	33.8 (1)	-	33.8	-	-	dyn/cm
Thermal Conductivity	-	158 (1)	-	158	-	-	mW/(m*K)
Vapor Pressure	3.45e-01 (1)	5.21e-01 (4)	3.45e-01	5.21e-01	3.45e-01	1.71e-01 to 9.99e-01	mmHg
Viscosity	-	3.61 (1)	-	3.61	-	-	cP
LogKoa: Octanol-Air	-	3.84 (1)	-	3.84	-	-	-
Henry's Law	3.20e-09 (1)	9.15e-09 (1)	3.20e-09	9.15e-09	-	-	atm-m ³ /mole
Index of Refraction	-	1.47 (1)	-	1.47	-	-	-
Molar Weight	-	226 (1)	-	226	-	-	g/mol

Chemical Properties

Env. Fate/Transport

Toxicity Values (Beta)

ADME (Beta)

Exposure

Bioassays

Similar Molecules (Beta)

Synonyms

Literature

External Links

Available Properties

- Solubility
 - Melting Point
 - Boiling Point
 - LogP (Octanol-water partition coefficient)
 - Atmospheric Hydroxylation Rate
 - LogBCF (Bioconcentration Factor)
 - Biodegradation Half-life
 - Henry's Law Constant
 - Fish Biotransformation Half-life
 - LogKOA (Octanol/Air Partition Coefficient)
 - LogKOC (Soil Adsorption Coefficient)
 - Vapor Pressure
-
- Data and models are updated ~90 days

Multiple Prediction Algorithms

Summary

LogP: Octanol-Water

Water Solubility

Density

Flash Point

Melting Point

Boiling Point

Surface Tension

Thermal Conductivity

Vapor Pressure

Viscosity

LogKoa: Octanol-Air

Henry's Law

LogP: Octanol-Water			
	Average	Median	Range
Experimental	-0.380 (1)	-0.380	-0.380
Predicted	-0.329 (5)	-0.329	-0.494 to -0.110

Download as: TSV Excel SDF

Experimental			
Source	Result		
PhysPropNCCT	-0.380		

Predicted			
Source	Result	Calculation Details	QMRF
EPISUITE	-0.110	Not Available	Not Available
NICEATM	-0.494	Not Available	Available
ACD/Labs Consensus	-0.345	Not Available	Not Available
ACD/Labs	-0.398	Not Available	Not Available
OPERA	-0.300	OPERA Model Report	Available

Consuming and Curating Public Data

Public data should be curated prior to modeling

Mol Block	CAS	NAME	Smiles
	000056-93-9	BENZYL TRIMETHYL AMMONIUM CHLORIDE	<chem>CN(C)(C)Cc1ccccc1.[Cl-]</chem>
	000068-05-3	TETRAETHYL AMMONIUM IODIDE	<chem>CC[N+](CC)(CC)CC.[I-]</chem>
	000071-91-0	TETRAETHYL AMMONIUM BROMIDE	<chem>CC[N+](CC)(CC)CC.[Br-]</chem>

Covalent Halogens

Structure	Formula	FIV	CAS	NAME	MP	EgMP	ErrorMP
	C ₃ H ₅ O ₃	90.0779	000050-21-5	LACTIC ACID	1.8200000000000000e+001	2.2860000000000000e+001	5.8800000000000000e+000
	C ₃ H ₅ O ₃	90.0779	000079-33-4	L-LACTIC ACID	5.3000000000000000e+001	2.2860000000000000e+001	-3.0340000000000000e+001
	C ₃ H ₅ O ₃	90.0779	000598-02-3	A-HYDROXYPROPIONIC ACID	1.8000000000000000e+001	2.2060000000000000e+001	4.6000000000000000e+000
	C ₃ H ₅ O ₃	90.0779	010328-41-7	D-LACTIC ACID	5.2800000000000000e+001	2.2860000000000000e+001	-3.0140000000000000e+001

Identical Chemicals

Mol Block	CAS	NAME	Smiles
	000076-43-7	FLUOXYMESTERONE	<chem>CC12CCC3C(C1CC2=O)C(=O)C(F)C3</chem>
	000077-99-6	1,1,1-TRIS(4-HYDROXYMETHYL)PROPANE	<chem>OC(CO)C(CO)CO</chem>
	000079-60-7	CORTISONE-99-FLUORO	<chem>CC12CCC3C(C1CC2=O)C(=O)C(F)C3</chem>
	000082-38-2	DISPERSE RED 9	<chem>CNc1ccc2c(c1)c(=O)c3ccccc3c2=O</chem>

Mismatches



Journal

SAR and QSAR in Environmental Research >

Volume 27, 2016 - Issue 11: 17th International Conference on QSAR in Environmental and Health Sciences (QSAR 2016) - Part II. Guest Editors: C.G. Barber and G.J. Myatt

258

Views

4

CrossRef citations

16

Altmetric

Articles

An automated curation procedure for addressing chemical errors and inconsistencies in public datasets used in QSAR modelling \$

K. Mansouri, C. M. Grulke, A. M. Richard, R. S. Judson & A. J. Williams 

Pages 911-937 | Received 03 Sep 2016, Accepted 24 Oct 2016, Published online: 25 Nov 2016

 Download citation

 <http://dx.doi.org/10.1080/1062936X.2016.1253611>

 Check for updates

OPERA on GitHub

GitHub navigation bar: This repository Search Pull requests Issues Marketplace Gist [Notifications] [User Profile]

kmansouri / OPERA

Unwatch 1 Unstar 1 Fork 0

Code Issues 0 Pull requests 0 Projects 0 Wiki Insights

Command line application providing QSAR models predictions as well as applicability domain and accuracy assessment for physicochemical properties and environmental fate endpoints.

36 commits 1 branch 0 releases 1 contributor MIT

Branch: master New pull request Create new file Upload files Find file Clone or download

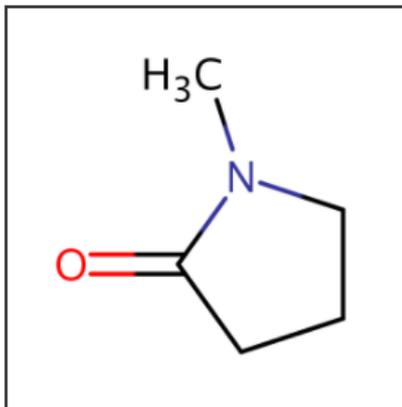
kmansouri committed on GitHub OPERA 1.2 Windows Latest commit 731deaf on May 19

Icon.png	OPERA 1.2 icon	3 months ago
LICENSE	Initial commit	9 months ago
Logo.png	Added logo and icon	9 months ago
Matlab_Source_code.tar.gz	OPERA 1.2 MATLAB source code	3 months ago
OPERA_CLI_Linux.tar.gz	OPERA 1.2 Linux	3 months ago
OPERA_CPP_library.tar.gz	OPERA 1.2 C++ Library	3 months ago
OPERA_C_library.tar.gz	OPERA 1.2 C Library	3 months ago

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

N-Methyl-2-pyrrolidone

872-50-4 | DTXSID6020856



Model Results

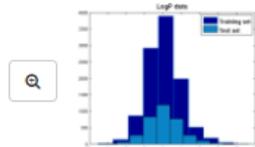
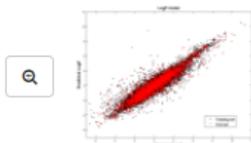
Predicted value: -0.300

Global applicability domain: inside ⓘ

Local applicability domain index: 0.88 ⓘ

Confidence level: 0.81 ⓘ

Model Performance

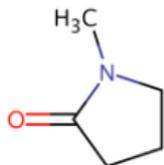


Weighted KNN model

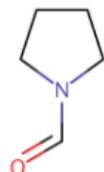
QMRf

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.88	0.67	0.88	0.78

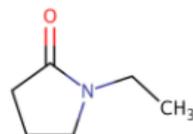
Nearest Neighbors from the Training Set



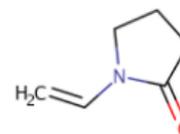
N-Methyl-2-pyrrolidone
 Measured: -0.380
 Predicted: -0.300



Proinal
 Measured: -0.320
 Predicted: -0.226

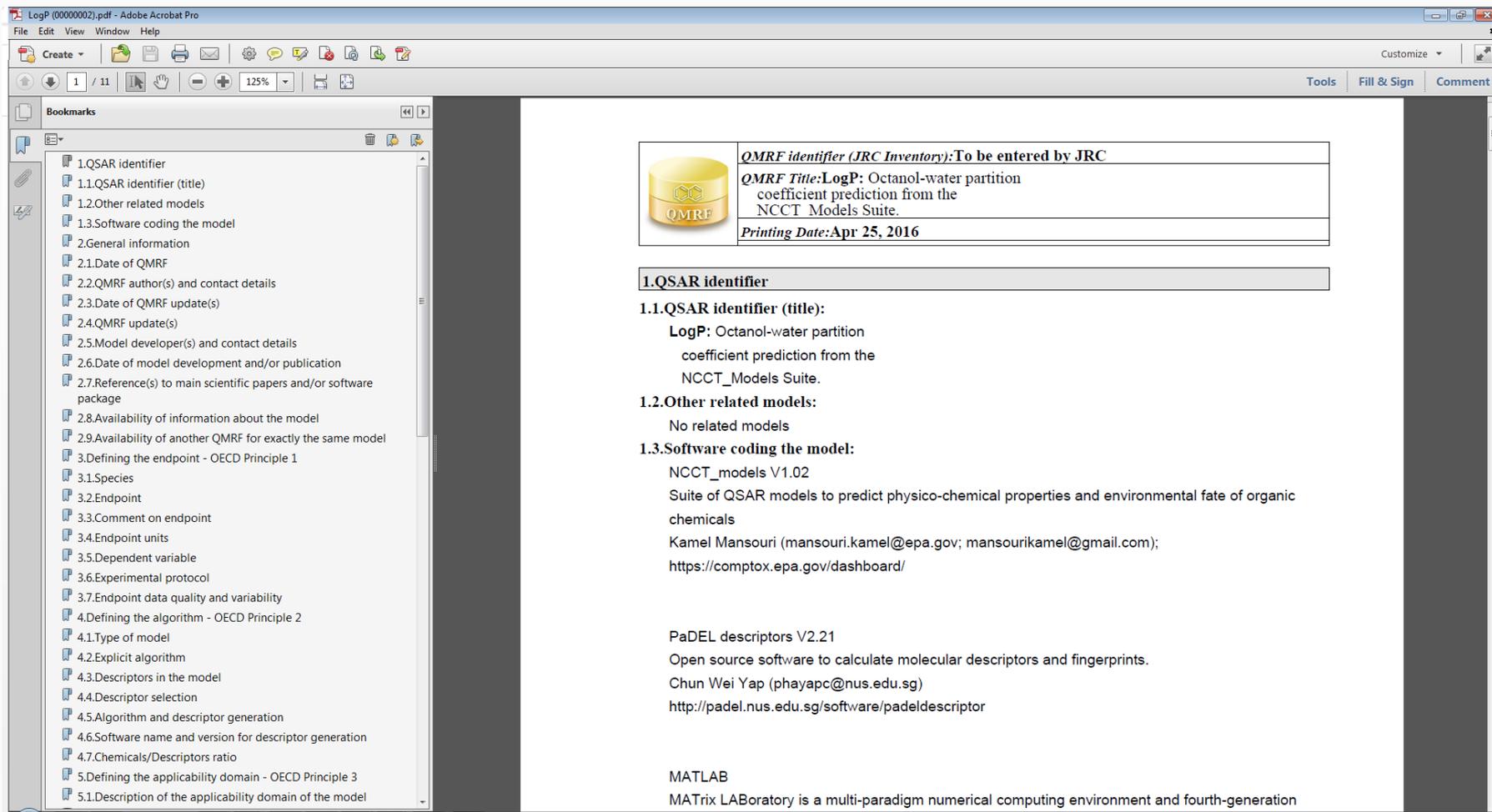


1-Ethyl-2-pyrrolidinone
 Measured: -0.0400
 Predicted: -0.211



N-Vinyl-2-pyrrolidone
 Measured: 0.37
 Predicted: 2.65e-01

QSAR Modeling Reporting Format



LogP (00000002).pdf - Adobe Acrobat Pro

File Edit View Window Help

Create [Icons]

1 / 11 125%

Tools Fill & Sign Comment

Bookmarks

- 1. QSAR identifier
 - 1.1. QSAR identifier (title)
 - 1.2. Other related models
 - 1.3. Software coding the model
- 2. General information
 - 2.1. Date of QMRP
 - 2.2. QMRP author(s) and contact details
 - 2.3. Date of QMRP update(s)
 - 2.4. QMRP update(s)
 - 2.5. Model developer(s) and contact details
 - 2.6. Date of model development and/or publication
 - 2.7. Reference(s) to main scientific papers and/or software package
- 2.8. Availability of information about the model
- 2.9. Availability of another QMRP for exactly the same model
- 3. Defining the endpoint - OECD Principle 1
 - 3.1. Species
 - 3.2. Endpoint
 - 3.3. Comment on endpoint
 - 3.4. Endpoint units
 - 3.5. Dependent variable
 - 3.6. Experimental protocol
 - 3.7. Endpoint data quality and variability
- 4. Defining the algorithm - OECD Principle 2
 - 4.1. Type of model
 - 4.2. Explicit algorithm
 - 4.3. Descriptors in the model
 - 4.4. Descriptor selection
 - 4.5. Algorithm and descriptor generation
 - 4.6. Software name and version for descriptor generation
 - 4.7. Chemicals/Descriptors ratio
- 5. Defining the applicability domain - OECD Principle 3
 - 5.1. Description of the applicability domain of the model

	QMRP identifier (JRC Inventory): To be entered by JRC
	QMRP Title: LogP: Octanol-water partition coefficient prediction from the NCCT Models Suite.
	Printing Date: Apr 25, 2016

1. QSAR identifier

1.1. QSAR identifier (title):
LogP: Octanol-water partition coefficient prediction from the NCCT_Models Suite.

1.2. Other related models:
No related models

1.3. Software coding the model:
NCCT_models V1.02
Suite of QSAR models to predict physico-chemical properties and environmental fate of organic chemicals
Kamel Mansouri (mansouri.kamel@epa.gov; mansourikamel@gmail.com);
<https://comptox.epa.gov/dashboard/>

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>

MATLAB
MATrix LABORatory is a multi-paradigm numerical computing environment and fourth-generation

Toxicity Values

Bioavailability Metric

Exposure Limit

Point Of Departure

Regulatory Toxicity Value

Effect Level

Misc Hazard Information

Screening Level

Uncertainty Factor

Download as:

TSV

Excel

Type	Subtype	Value	Units	Study Type	Exposure Route	Study Duration	Species	Media	Details	Source
TD50	-	20.7	mM/kg-day	-	-	-	-	-	DSSTox C...	ACToR
TD50	-	2050	mg/kg-day	-	-	-	-	-	DSSTox C...	ACToR
LEL	systemic	619	mg/kg-day	subchronic	oral	subchronic	mouse	-	Study ID: ...	ToxRefDB
NEL	systemic	277	mg/kg-day	subchronic	oral	subchronic	mouse	-	Study ID: ...	ToxRefDB
LEL	systemic	25.0	mg/kg-day	subchronic	oral	subchronic	dog	-	Study ID: ...	ToxRefDB
NEL	systemic	25.0	mg/kg-day	subchronic	oral	subchronic	dog	-	Study ID: ...	ToxRefDB
LEL	systemic	173	mg/kg-day	chronic	oral	chronic	mouse	-	Study ID: ...	ToxRefDB
NEL	systemic	115	mg/kg-day	chronic	oral	chronic	mouse	-	Study ID: ...	ToxRefDB
LEL	systemic	678	mg/kg-day	chronic	oral	chronic	rat	-	Study ID: ...	ToxRefDB
NEL	systemic	283	mg/kg-day	chronic	oral	chronic	rat	-	Study ID: ...	ToxRefDB
LEL	systemic	1230	mg/kg-day	subacute	oral	subacute	rat	-	Study ID: ...	ToxRefDB
NEL	systemic	493	mg/kg-day	subacute	oral	subacute	rat	-	Study ID: ...	ToxRefDB
LEL	systemic	2130	mg/kg-day	subacute	oral	subacute	mouse	-	Study ID: ...	ToxRefDB
NEL	systemic	920	mg/kg-day	subacute	oral	subacute	mouse	-	Study ID: ...	ToxRefDB



National Health and Nutrition Examination Survey

High-Throughput Models for Exposure-Based Chemical Prioritization in the ExpoCast Project

Environ. Sci. Technol., **2013**, 47 (15), pp 8479–8488



Product & Use Categori...

Chemical Weight Fraction

Chemical Functional Use

Monitoring Data

Exposure Predictions

Download as:

National Health and Nutrition Examination Survey (NHANES) Inferences (mg/kg-bw/day)

	Lower 95th Limit	Upper 95th Limit	Median
Ages 6-11	3.80e-05	4.92e-05	4.33e-05
Ages 12-19	2.55e-05	3.38e-05	2.93e-05
Ages 20-65	2.79e-05	3.27e-05	3.02e-05
Ages 65+	1.91e-05	2.31e-05	2.10e-05
BMI > 30	2.38e-05	2.74e-05	2.55e-05
BMI < 30	3.02e-05	3.30e-05	3.16e-05
Repro. Age Females	2.83e-05	3.31e-05	3.06e-05
Females	2.58e-05	3.03e-05	2.80e-05
Males	2.94e-05	3.37e-05	3.15e-05
Total	2.86e-05	3.08e-05	2.97e-05

Chemical Properties

Env. Fate/Transport

Synonyms

External Links

Toxicity Values (Beta)

Exposure

Bioassays

Similar Molecules (Beta)

Literature

Comments

Product Composition Details

Chemical Weight Fractions

Download as:

Product Name	Product Use Category	Minimum Weight Fraction	Maximum Weight Fraction	Data Type	Source
citristrip canadian stripping...	home maintenance: stripper	0.65	0.7	MSDS	Retail Product Categories/...
citristrip stripping gel qog7...	home maintenance: stripper	0.4	0.55	MSDS	Retail Product Categories/...
gumout 2 part professional...	auto products: auto fluids a...	0.3	0.4	MSDS	Retail Product Categories/...
minwax water based wipe ...	home maintenance: finish	0.06	0.06	MSDS	Retail Product Categories/...
10-02199- calico tip & glue...	personal care: nail polish r...	0.01	0.05	MSDS	Retail Product Categories/...
artificial nail remover 728 1	personal care: nail polish r...	0.01	0.05	MSDS	Retail Product Categories/...
calico tip & glue remover 1	personal care: nail polish r...	0.01	0.05	MSDS	Retail Product Categories/...
kiss nail remover 1	personal care: nail polish r...	0.01	0.05	MSDS	Retail Product Categories/...
waterborne clear wood fini...	home maintenance: finish	0.01	0.05	MSDS	Retail Product Categories/...

[Chemical Properties](#)

[Env. Fate/Transport](#)

[Toxicity Values \(Beta\)](#)

[ADME \(Beta\)](#)

[Exposure](#)

[Bioassays](#)

[Similar Molecules \(Beta\)](#)

[Synonyms](#)

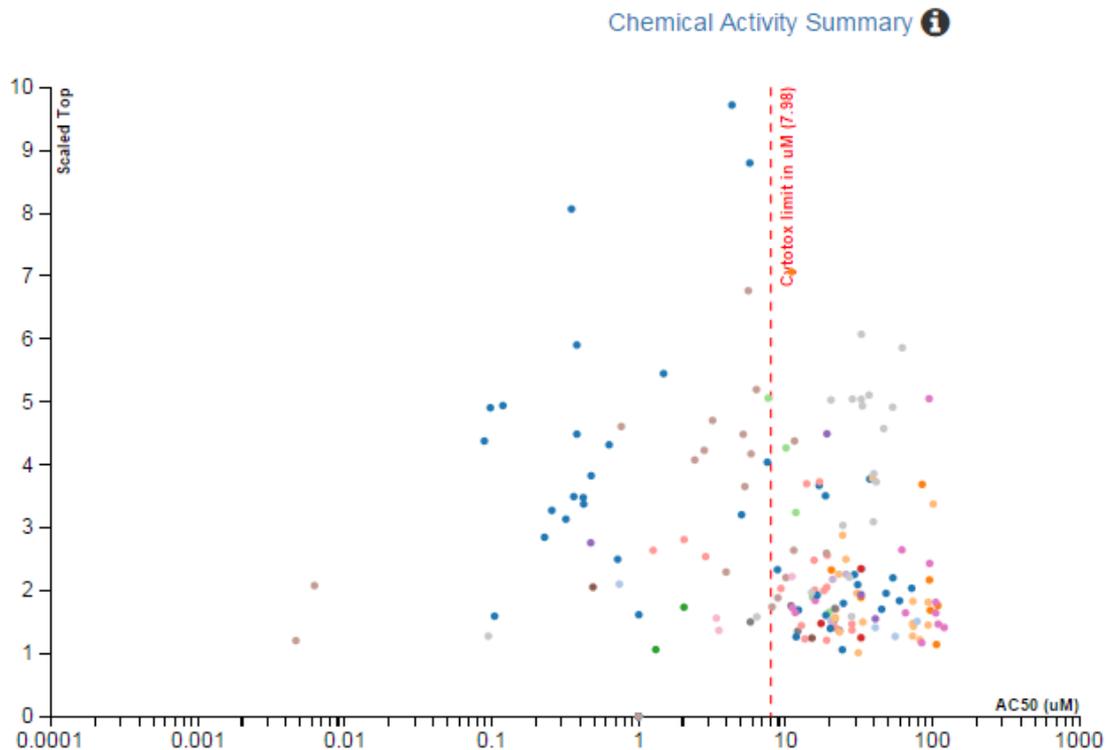
[Literature](#)

[External Links](#)

ToxCast and Tox21 Bioassays

ToxCast

- PubChem
- ScrubChem (Beta)



- Show/Hide All
- nuclear receptor
 - background measurement
 - cell morphology
 - dna binding
 - steroid hormone
 - transporter
 - ion channel
 - gpcr
 - oxidoreductase
 - kinase
 - protease
 - cyp
 - cell cycle
 - cytokine
 - cell adhesion molecules
 -

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Similar Molecules (Beta)

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Comments

ToxCast and Tox21 Bioassays

Download as:

TSV

Excel

Show:

Inactive

Background

Assay Name	Hit Call	Top	Scaled Top	AC50	log AC50 ↓	Intended Target Family
APR_Hepat_CellLoss_48hr_dn	ACTIVE	1.41	1.41	120	2.08	cell cycle
APR_HepG2_MitoMass_24h_dn	ACTIVE	0.874	1.76	109	2.04	cell morphology
APR_HepG2_OxidativeStress_24h_up	ACTIVE	1.20	1.47	110	2.04	cell cycle
APR_Hepat_DNADamage_48hr_up	ACTIVE	1.84	1.14	107	2.03	cell morphology
APR_HepG2_CellLoss_24h_dn	ACTIVE	1.20	1.81	106	2.02	cell cycle
APR_HepG2_OxidativeStress_72h_up	ACTIVE	1.80	1.65	106	2.02	cell cycle
ATG_HSE_CIS_up	ACTIVE	1.59	3.38	102	2.01	dna binding

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Literature

Comments

Names and Identifiers

Found 40 synonyms

Legend: **Valid Synonyms** *Good Synonyms* Other Synonyms

 Copy all Synonyms

N-Methyl-2-pyrrolidone

1-Methylpyrrolidin-2-one

2-Pyrrolidinone, 1-methyl-

872-50-4 Active CAS-RN

2-Pyrrolidinone, 1-methyl-

1-Methyl-2-pyrrolidinone

1-Methyl-2-pyrrolidon

1-Methyl-2-pyrrolidone

1-Methyl-5-pyrrolidinone

1-Methylazacyclopentan-2-one

1-Methylpyrrolidone

1-metil-2-pirrolidona

2-Pyrrolidinone, 1-methyl-

2-Pyrrolidone, 1-methyl-

Microposit 2001

M-Pyrol

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Integrated Literature Searching

Google Scholar

PubMed Abstract S...

PubChem Articles

PubChem Patents

Select Term:

Hazard

AND

RfD OR reference dose



"RfD OR reference dose" AND "Hazard" AND "872-50-4" OR "N-Methyl-2-py



Scholar

About 22 results (0.05 sec)

Articles

[Solvent Substitution: An Analysis of Comprehensive Hazard Screening Indices](#)

M Debia, D Bégin, M Gérin - *Journal of occupational and ...*, 2011 - oeh.tandfonline.com

Case law

... Reliability and weighting factors were not used. Armenti and Moure-Eraso(22) used the same FHS index, using six **hazard** categories, to compare replacement options. ...

My library

872-50-4 N-Methyl-2-pyrrolidone 45.4 13 1.46E-03 11 4.55 6 20 4 ...

[Related articles](#) [All 4 versions](#) [Cite](#) [Save](#)

Any time

[Effects of 'inactive'ingredients on bees](#)

Since 2017

[CA Mullin](#) - *Current Opinion in Insect Science*, 2015 - Elsevier

Since 2016

... tallow amines, organosilicone ethoxylates and co-solvents such as **N-methyl-2-pyrrolidone** (NMP)

Since 2013

[7 ... of tools to environmentally monitor residues and determine their relative **hazard** to bees. ... Defining a benchmark or **reference dose**, particularly for bee viruses [51], for what can ...

Custom range...

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WM Draper - *Analytical chemistry*, 2001 - ACS Publications

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[Evolution of chemical-specific adjustment factors \(CSAF\) based on recent international experience; increasing utility and facilitating regulatory acceptance](#)

VS Bhat, ME Meek, M Valcke, C English... - *Critical Reviews in ...*, 2017 - Taylor & Francis

... As shown in the right side of Figure 2, uncertainty is taken into consideration at all tiers of **hazard** assessment. ... For decades, developing "safe doses" such as the oral **reference dose** (RfD), the inhaled reference concentration (RfC) or the acceptable or tolerable daily intake (ADI ...

[All 3 versions](#) [Cite](#) [Save](#)

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Integrated Literature Searching

Google Scholar

PubMed Abstract ...

PubChem Articles

PubChem Patents

Select Term:

Select a Query Term

Select a Query Term

Hazard

Fate and Transport

Metabolism/PK/PD

Chemical Properties

Exposure

Mixtures

Male Reproduction

Androgen Disruption

Female Reproduction

GeneTox

Embryo and embryonic development

Child (infant through adolescent)

Dust and Exposure

ng Articles

rrolidone" OR "N-methylpyrrolidone"

Search and Count

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Google Scholar

PubMed Abstract Sifter

PubChem Articles

PubChem Patents

Edit the Query Before Retrieving Articles

```
("872-50-4" OR "N-Methyl-2-pyrrolidone" OR "N-methylpyrrolidone") AND (exposure OR near-field OR far-field OR SHEDS[tiab] AND ENVIRONMENTAL MONITORING)
```

1

0

0	0	0	0	24078144	2013	Biological monitoring and health effects of low-level exposure to N-methyl-2-pyrrolidone: a cross-sectional study.
0	0	0	0	23337464	2013	Biomonitoring of exposure to N-methyl-2-pyrrolidone in workers of the automobile industry.
0	0	0	0	19875680	2009	Quantitative risk analysis for N-methyl pyrrolidone using physiologically based pharmacokinetic and benchmark dos...
0	0	0	0	16897094	2006	Human volunteer study on the influence of exposure duration and dilution of dermally applied N-methyl-2-pyrrolidon...

Record:   1 of 16  

Title: [Not Available].

Abstract: N-Ethyl-2-pyrrolidone (NEP), a polar aprotic solvent, is used in many applications as substitute for the structural analogue N-methyl-2-pyrrolidone (NMP), e. g. for surface coatings, in cleaning agents and paint strippers. Monitoring studies indicate that individuals within the general public, without occupational exposure, may be exposed to NEP to an extent, which is comparable to NMP. As NMP, NEP presents a potential health hazard due to its developmental toxicity and teratogenicity. Exposure to NEP can be quantified by the determination of the excretion of its urinary metabolites 5-Hydroxy-N-ethyl-2-pyrrolidone (5-HNEP) and 2-Hydroxy-N-ethylsuccinimide (2-HESI). For the derivation of HBM values, the German Human Biomonitoring Commission (HBM Commission) evaluated different toxicological endpoints and finally decided on the BMDL05 and the BMD10 for the endpoint "reduced grasp intensity" of a subchronic feeding study with rats as point of departure (POD) for further procedural steps. The resulting HBM-I and HBM-II values for the sum of the metabolites 5-HNEP and 2-HESI in the urine of children are 10 resp. 25 mg/l and in the urine of adults are 15 resp. 40 mg/l. If the HBM values are exceeded, a check-up will be necessary at first. Measurements above the HBM-II value give cause for concern, especially for pregnant women. Air measurements to determine the source of exposure can be useful. The possibility of skin absorption from use of

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Pubmed Abstract Sifter

Select Term:

Exposure

Retrieve Articles

0 Articles

Add additional query terms to filter abstracts:

developmental

reproductive

occupational

Search and Count

Edit the Query Before Retrieving Articles

("872-50-4" OR "N-Methyl-2-pyrrolidone" OR "N-methylpyrrolidone") AND (exposure OR near-field OR far-field OR SHEDS[tiab] AND ENVIRONMENTAL MONITORING)

dev...	rep...	occ...	Total	PMID	Pu...	Title
0	0	1	1	24078144	2013	Biological monitoring and health effects of low-level exposure to N-methyl-2-pyrrolidone: a cross-sectional study.
1	0	0	1	23337464	2013	Biomonitoring of exposure to N-methyl-2-pyrrolidone in workers of the automobile industry.
0	0	2	2	19875680	2009	Quantitative risk analysis for N-methyl pyrrolidone using physiologically based pharmacokinetic and benchmark dos...
0	0	1	1	16897094	2006	Human volunteer study on the influence of exposure duration and dilution of dermally applied N-methyl-2-pyrrolidon...
0	0	0	0	16362322	2005	Ambient monitoring and biomonitoring of workers exposed to N-methyl-2-pyrrolidone in an industrial facility

Record: 1 of 16

Title: Stillbirth after occupational exposure to N-methyl-2-pyrrolidone. A case report and review of the literature.

Abstract: N-methyl-2-pyrrolidone is a solvent that is increasingly used in a variety of industries, including petroleum refining, microelectronics, pesticide formulation, and veterinary medicine. Animal studies have demonstrated fetotoxic effects after maternal exposure to doses that have minimal to no adverse effect on the mothers. The fetotoxicity comprises resorption, stillbirth, and low birthweight and delayed ossification in surviving young. We report a human case of intrauterine growth retardation followed by fetal demise at 31 weeks gestation. The mother was a laboratory worker with no other apparent risk factors, who sustained occupational exposure to N-methyl-2-pyrrolidone throughout the first trimester of pregnancy. Laboratory work and solvent exposure have both previously been associated with adverse reproductive outcomes. Laboratories and other industries that use suspected reproductive toxins should have reproductive health policies in place that allow for decision-making based on toxicologic review, exposure assessment, and medical evaluation. These policies should allow for voluntary removal of prospective parents until environmental assessment and controls are instituted.

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Links to Other Resources

General

-  EPA Substance Re...
-  NIST Chemistry W...
-  Household Product...
-  PubChem
-  Chempider
-  CPCat
-  DrugBank
-  HMDB
-  Wikipedia
-  MSDS Lookup
-  ChEMBL
-  Chemical Vendors
-  Consumer Product...

Toxicology

-  ACToR
-  DrugPortal
-  CCRIS
-  ChemView
-  CTD
-  EPA
-  GHS
-  HSDB
-  ToxCast Dashboar...
-  LactMed
-  ACToR PDF Report
-  International Toxicit...

Publications

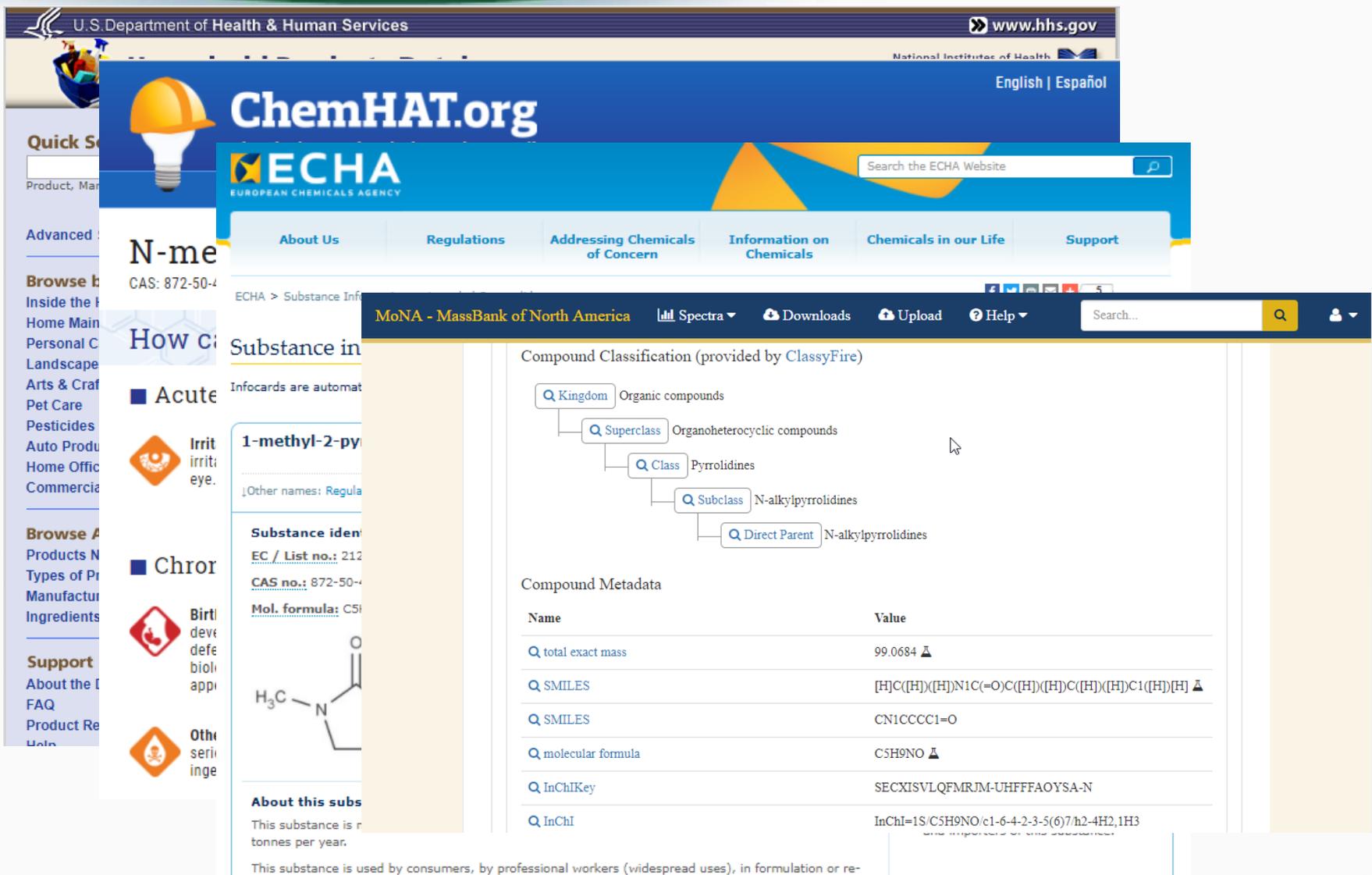
-  Toxline
-  Environmental Heal...
-  NIEHS
-  National Toxicology...
-  Google Books
-  Federal Register
-  Regulations.gov
-  Springer Materials
-  BioCaddie DataMed
-  RSC Publications

Analytical

-  National Environme...
-  MONA: MassBank ...
-  Tox21 Analytical Data
-  RSC Analytical Abs...
-  FOR-IDENT

The Office of the Federal Register (OFR) of the National Archives and Records Administration (NARA), and the U.S. Government Printing Office (GPO) jointly administer the FederalRegister.gov website.

Example External Links...



The screenshot displays the ChemHAT.org website interface, which is a hub for chemical safety information. It features a navigation menu with categories such as 'About Us', 'Regulations', 'Addressing Chemicals of Concern', 'Information on Chemicals', 'Chemicals in our Life', and 'Support'. A search bar is prominently displayed at the top right of the main content area.

Two external links are highlighted:

- ECHA (European Chemicals Agency):** The link leads to a page for 'N-methyl-2-pyrrolidone' (CAS: 872-50-4). The page includes a 'Substance information' section with details on acute and chronic effects, and a 'Compound Classification' section provided by ClassyFire.
- MoNA - MassBank of North America:** This link provides a detailed view of the compound's classification and metadata.

Compound Classification (provided by ClassyFire):

- Kingdom: Organic compounds
- Superclass: Organoheterocyclic compounds
- Class: Pyrrolidines
- Subclass: N-alkylpyrrolidines
- Direct Parent: N-alkylpyrrolidines

Compound Metadata:

Name	Value
total exact mass	99.0684
SMILES	[H]C([H])([H])N1C(=O)C([H])([H])C([H])([H])C1([H])[H]
SMILES	CN1CCCC=O
molecular formula	C5H9NO
InChIKey	SECXISVLQFMRJM-UHFFFAOYSA-N
InChI	InChI=1S/C5H9NO/c1-6-4-2-3-5(6)/h2-4H2,1H3

- Build out definitive “lists” of chemicals
 - Algal toxins
 - Poly/perfluorinated chemicals
 - Pesticides
 - Toxcast screening chemical collection
 - Public data sets:
 - NORMAN Network data collections
 - MASSBANK data

The Collection of Lists

Chemistry Dashboard

NIOSH Skin Notation Profiles

57

The NIOSH skin notations relies on multiple skin notations to provide users a warning on the direct, systemic, and sensitizing effects of exposures of the skin to chemicals.

NORMAN Collaborative Trial 2015 Targets and Suspects 732

NORMANCT15 is a compilation of all target and suspect substances reported by participants in the **NORMAN** Collaborative Trial on Non-target Screening, run by the **NORMAN** Network and described in Schymanski et al 2015, DOI: 10.1007/s00216-015-8681-7

Chemistry Dashboard | NORMANEWS

NormaNEWS: Norman Early Warning System

Search NORMANEWS Chemicals



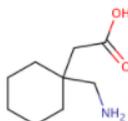
List Details

Description: The Norman Early Warning System (NormaNEWS) is a pilot network designed to investigate the spatial and temporal distribution of newly identified contaminants of emerging concern in environmental samples through performing retrospective suspect screening on HRMS data acquired using different instrumental platforms and data processing software. The NormaNEWS pilot study was performed through recruiting eight reference laboratories with available archived HRMS data with the goal of exploring the potential of an early warning network to rapidly establish the occurrence of newly-identified contaminants of emerging concern across Europe and beyond, through the use of retrospective suspect screening employing HRMS. The pilot study was referred to as the Norman Early Warning System, abbreviated to NormaNEWS.

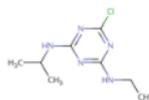
Number of Chemicals: 131

Sort Options Select/Deselect All Download as: TSV Excel SDF

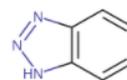
View Selected



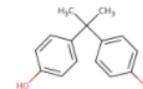
Gabapentin
60142-96-3



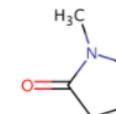
Atrazine
1912-24-9



1,2,3-Benzotriazole
95-14-7



Bisphenol A
80-05-7



N-Methyl-2-pyrrolidone
872-50-4



Batch Searching for Data for Thousands of Chemicals

- What are these chemicals?

**Chemicals Used in the Hydraulic Fracturing Process in Pennsylvania
Prepared by the Department of Environmental Protection
Bureau of Oil and Gas Management**

Updated June 10, 2010

Chemical	Product Name
2,2-Dibromo-3-Nitrilopropionamide	Bio Clear 1000/Bio Clear 2000/ Bio-Clear 200/BioRid20L/ EC6116A
2-methyl-4-isothiazolin-3-one	X-Cide 207
5-chloro-2-methyl-4-isothiazolin-3-one	X-Cide 207
Acetic Acid	Fe-1A Acidizing Composition/ Packer Inhibitor
Acetic Anhydride	Fe-1A Acidizing Composition
Acetylene	GT&S Inc./ Airco
Alcohol Ethoxylated	C12-16 NE-200
Alkyl benzene sulfonic acid	Tetrolite AW0007/ FR-46
Ammonia (aqueous)	FAW-5
Ammonium Bifluoride	ABF 37%
Ammonium Persulfate	AP Break
Ammonium Bisulfite	Techni-Hib 604/ Fe OXCLEAR/ Packer Inhibitor
Ammonium chloride	Salt Inhibitor
Ammonium Salt (alkylpolyether	

Batch Searching for Data for Thousands of Chemicals

Select Input Type(s)

- Chemical Name
- CAS-RN
- InChIKey
- DSSTox Substance ID
- Exact Molecular Formula ⓘ

Enter Identifiers to Search

Sodium l-glutamate
4-Hydroxy-3-nitrophenylarsonic acid
4-Nitro-1,2-phenylenediamine
Methoxypromazine
1-Phenyl-3-methyl-5-pyrazolone
1-Phenyl-2-thiourea
Phenylbutazone
1,4-Benzenediamine
Prednisolone
Probenecid

Display All Chemicals Download Chemical Data

Select Output Format

Excel ▼

Customize Results

Select All

Chemical Identifiers	Structures	Intrinsic Properties
<input checked="" type="checkbox"/> Chemical Name	<input type="checkbox"/> Mol File	<input type="checkbox"/> Molecular Formula
<input checked="" type="checkbox"/> DTXSID	<input type="checkbox"/> SMILES	<input type="checkbox"/> Average Mass
<input type="checkbox"/> CAS-RN	<input type="checkbox"/> InChI String	<input type="checkbox"/> Monoisotopic Mass
<input type="checkbox"/> InChIKey		<input type="checkbox"/> OPERA and TEST Model Predictions
<input type="checkbox"/> IUPAC Name		

Access to associated data for review, modeling & download

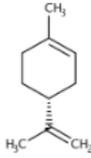
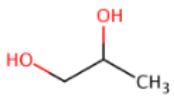
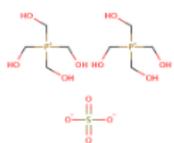
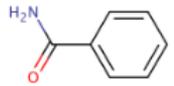
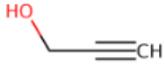
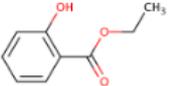
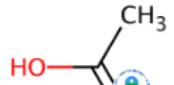
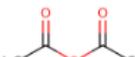
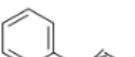
 United States Environmental Protection Agency

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Search Chemistry Dashboard

Chemistry Dashboard

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 <p>D-Limonene 5989-27-5</p>	$K^+ Cl^-$ <p>Potassium chloride 7447-40-7</p>	 <p>1,2-Propylene glycol 57-55-6</p>	$Na^+ O^- C(=O)OH$ <p>Sodium bicarbonate 144-55-8</p>	 <p>Tetrakis(hydroxymethyl)phospho... 55566-30-8</p>	
 <p>Benzamide 55-21-0</p>	H_3C-OH <p>Methanol 67-56-1</p>	 <p>1-Butanol 71-36-3</p>	 <p>Propargyl alcohol 107-19-7</p>	 <p>Ethyl salicylate 118-61-6</p>	
 <p>About</p>	 <p>Contact</p>	 <p>Privacy</p>	 <p>ACToR</p>	 <p>DSSTox</p>	
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 United States Environmental Protection Agency

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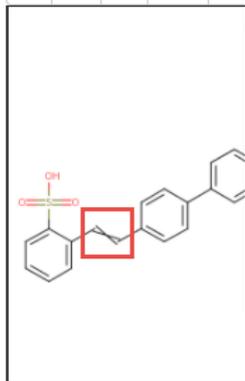
Search All Data

Chemistry Dashboard

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2,2'-[biphenyl-4,4'-
38775-22-3 | DTXSID7047

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New Comment

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Email address

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Presence in Lists

Record Information

Chemical Properties

Env. Fate/Transport

Toxicity Values (Beta)

ADME (Beta)

Exposure

Bioassays

Similar Molecules (Beta)

Synonyms

Literature

Crowdsourced Curation – **HELP!**

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

Chemical Properties Env. Fate/Transport Toxicity Values (Beta) ADME (Beta) Exposure Bioassays Similar Molecules (Beta) Synonyms Literature

External Links Comments

Add A Comment

Comment from structure source: to my knowledge the stilbene-derived fluorescent whitening agents are all trans (E) isomers, as the cis (Z) isomers are not fluorescent (although they might undergo photo-isomerisation to the cis isomers under UV light, and clothing gets yellowish again then...) . Thus I would consider the E,E form the correct one, although I don't know whether it is synthesized in a way that x % of the technical product are actually the inactive E,Z (dunno if this is still active?) or Z,Z forms and thus the undefined stereo would be correct. In the environment E,E is partly transformed to E,Z (maybe also Z,Z) and thus both isomers occur, see: <http://pubs.acs.org/doi/pdf/10.1021/es960748a> CAS number on record was 27344-41-8 which is DTXSID6036467.

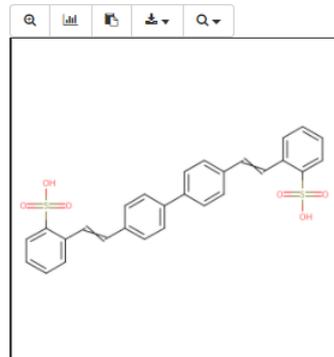
User comment posted 1 day ago

- The Question – is this a mixture of E/Z, E/E or Z/Z? Brighteners should be E/E...
- **Thanks for helping us Emma!**

Curation is laborious work

38775-22-3 | DTXSID7047017

© Searched by DSSTox_Substance_Id: Found 1 result for 'DTXSID7047017':



- So, it's clear what the correct E/Z orientation is yes???

CAS Registry Number 38775-22-3

~160  ~17 

C₂₈ H₂₂ O₆ S₂

Benzenesulfonic acid, 2,2'-([1,1'-biphenyl]-4,4'-diyldi-2,1-ethenediyl) bis-

Molecular Weight

518.60

Density (Predicted)

Value: 1.414±0.06 g/cm³ | Condition: Temp: 20 °C Press: 760 Torr

pKa (Predicted)

Value: -0.92±0.27 | Condition: Most Acidic Temp: 25 °C

Other Names

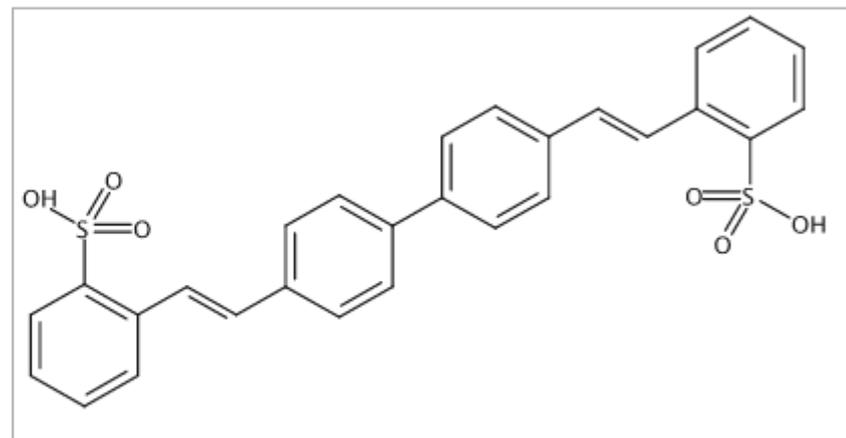
2,2'-([1,1'-Biphenyl]-4,4'-diyldi-2,1-ethenediyl)bis[benzenesulfonic acid]

4,4'-Bis(2-sulfoxyphenyl)biphenyl

4,4'-Bis[2-(2-sulfoxyphenyl)ethenyl]biphenyl

C.I. 482200

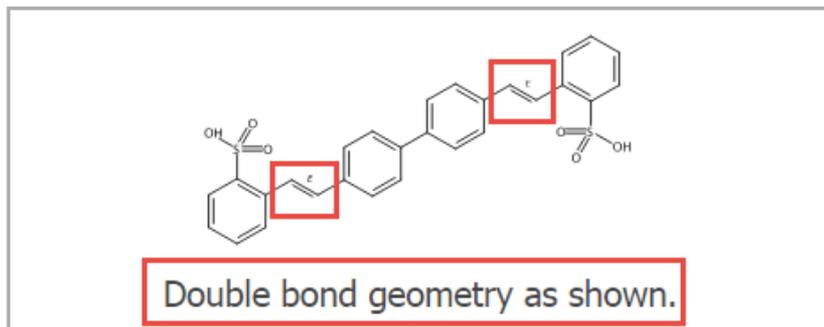
C.I. Fluorescent Brightener 351



Curation is laborious work

1. **334756-45-5** 🔍

~5 📄 ~1 🧪



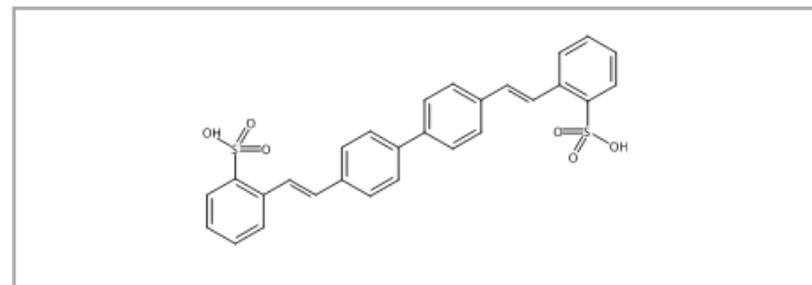
C₂₈ H₂₂ O₆ S₂

Benzenesulfonic acid, 2,2'-**(1E)**-[1,1'-biphenyl]-4,4'-diyldi-2,1-ethenediyl]bis- (9CI)

▶ **Key Physical Properties**

2. **38775-22-3** 🔍

~160 📄 ~17 🧪



C₂₈ H₂₂ O₆ S₂

Benzenesulfonic acid, 2,2'-([1,1'-biphenyl]-4,4'-diyldi-2,1-ethenediyl)bis-

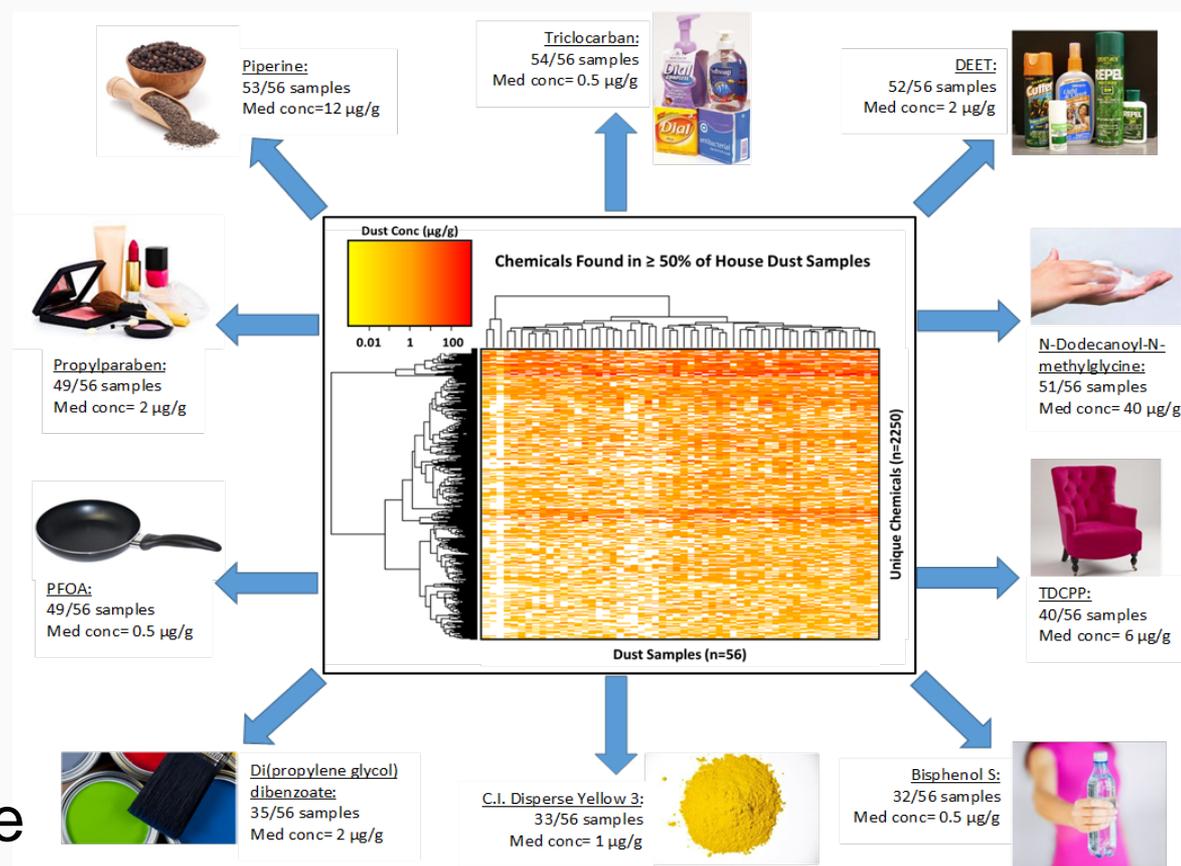
▶ **Key Physical Properties**

Regulatory Information

- I have a 1000 CAS Numbers (or Names) – is there data available?
 - Has any Toxcast data been run?
 - Are there Toxicity Data values available?
 - Are there predicted exposure data (via Expocast)?
 - Can I get predicted physchem data for my model?
- Identifying chemicals by analytical chemistry

Suspect Screening Analysis Chemicals in House Dust

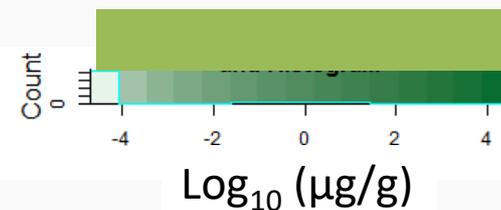
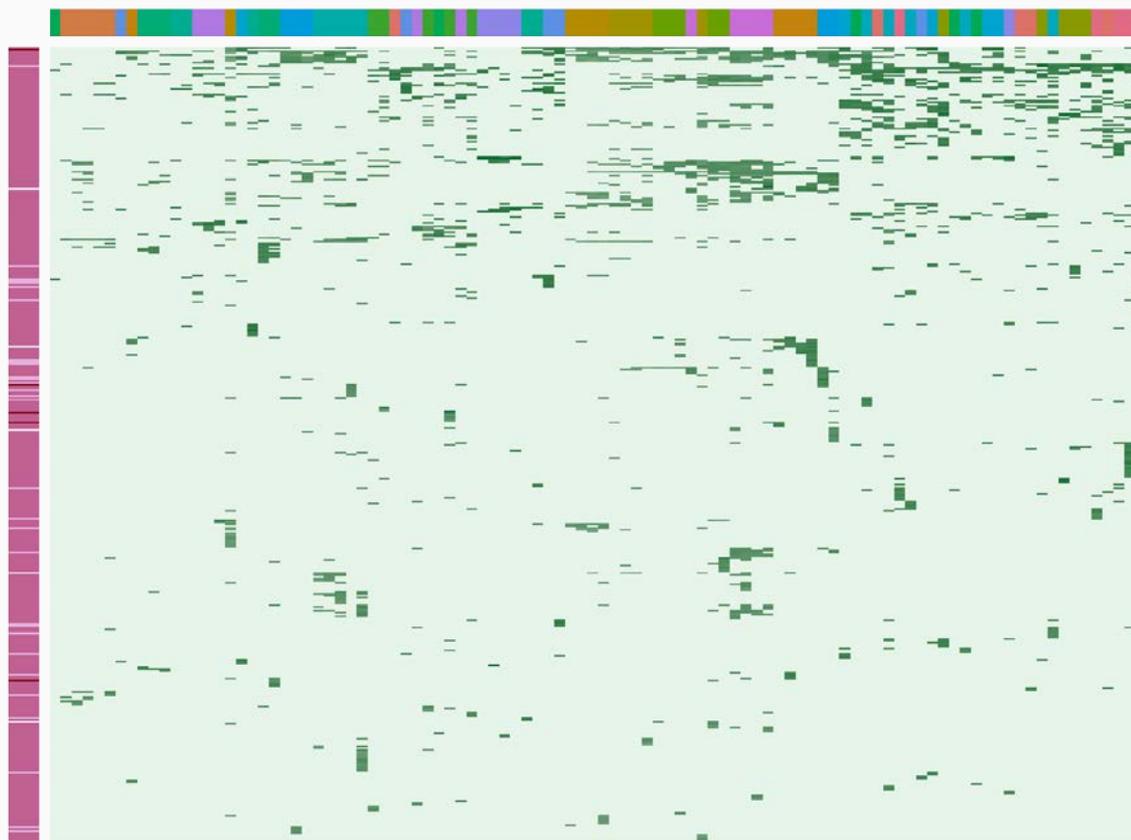
- Chemical confirmation from ToxCast
- Detection frequency
- External calibration for concentrations
- Cluster analysis (homes/chemicals)
- Chemical functional use



Improving Exposure Estimates – Characterizing Commercial Products

423 ToxCast and/or Commonly Occurring Chemicals*

100 Consumer Products and Articles of Commerce



- Air freshener
- Baby soap
- Carpet
- Carpet padding
- Cereals
- Cotton clothing
- Deodorant
- Fabric upholstery
- Glass cleaners
- Hand soap
- Indoor house paint
- Lipstick
- Plastic children's toys
- Shampoo
- Shaving cream
- Shower curtain
- Skin lotion
- Sunscreen
- Toothpaste
- Vinyl upholstery

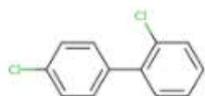
- GCXGC-MS with DCM Extraction
- 1606 tentative and confirmed chemical identifications

- Common Chemical (n>19)
- ToxCast
- Flame Retardant
- Potent ER

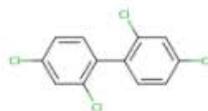
- Sometimes the simplest of questions are difficult to answer!
 - What is the list of CAS Numbers for all PCBs?
 - Can I get an SDF file of all PCBs?
 - Do you have predicted properties for all PCBs?
 - What toxicity data is available for individual PCBs?
 - Have you measured ToxCast data for any PCBs?
 - Can I get all PCBs listed in an Excel Spreadsheet?

Chemical "Families"

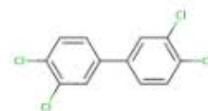
Download as: [TSV](#) [Excel](#) [SDF](#)



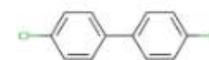
2,4'-Dichlorobiphenyl
34863-43-7



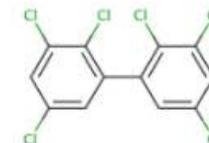
2,2',4,4'-Tetrachlorobiphenyl
2437-79-8



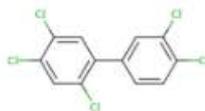
3,3',4,4'-Tetrachlorobiphenyl
32598-13-3



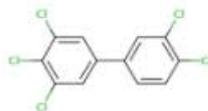
4,4'-Dichlorobiphenyl
2050-68-2



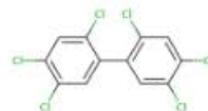
2,2',3,3',5,5'-Hexachlorobiphenyl
35694-04-3



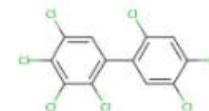
2,3',4,4',6-Pentachlorobiphenyl
31508-00-6



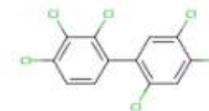
3,3',4,4',5-Pentachlorobiphenyl
57485-28-8



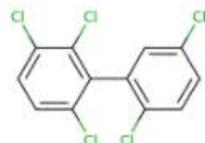
2,2',4,4',5,5'-Hexachlorobiphenyl
32065-27-1



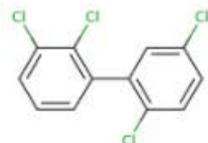
2,2',3,4,4',5,5'-Heptachlorobiphenyl
35065-29-3



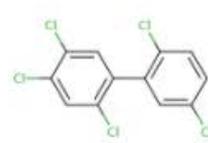
2,2',3,4,4',5'-Hexachlorobiphenyl
35065-28-2



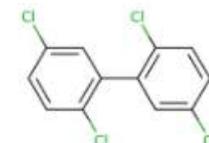
2,2',3,5',6-Pentachlorobiphenyl
36379-99-6



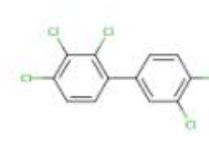
2,2',3,5'-tetrachlorobiphenyl
41464-39-5



2,2,4,5,5'-Pentachlorobiphenyl
37680-73-2



2,2',5,5'-Tetrachlorobiphenyl
35693-99-3



2,3,3',4,4'-Pentachlorobiphenyl
32598-14-4

One click download

A	B	C	D	E	F	G	H	I
DTXSID	CASRN	PREFERRED NAME	IUPAC NAME	MOLECULAR FORMULA	MONOISOTOPIC WEIGHT	AVERAGE WEIGHT	SMILES	INCHI KEY
DTXSID9074779	70362-45-7	PCB 045	2,2',3,6-Tetrachloro-1,1'-biphenyl	C12H6Cl4	289.92236	291.98001	C1C1=CC=C(C1)C(=C1)C1=CC=CC=C1C1	VHGHZT
DTXSID9074777	38444-73-4	PCB 019	2,2',6-Trichloro-1,1'-biphenyl	C12H7Cl3	255.96133	257.54001	C1C1=CC=CC(C1)=C1C1=C(C1)C=CC=C1	MXVJRBBC
DTXSID9074228	74472-39-2	2,3',4',5',6-Pentachlorobiphenyl	2,3',4',5',6-Pentachloro-1,1'-biphenyl	C12H5Cl5	323.88339	326.42001	C1C1=CC(=CC(C1)=C1)C1=C(C1)C=CC=C1C1	WAZUWHC
DTXSID9074226	74472-37-0	2,3,4,4',5-Pentachlorobiphenyl	2,3,4,4',5-Pentachloro-1,1'-biphenyl	C12H5Cl5	323.88339	326.42001	C1C1=CC=C(C=C1)C1=C(C1)C(C1)=C(C1)C(C1)=C1	SXZSFWHC
DTXSID9074224	74472-35-8	2,3,3',4,6-Pentachlorobiphenyl	2,3,3',4,6-Pentachloro-1,1'-biphenyl	C12H5Cl5	323.88339	326.42001	C1C1=CC=CC(=C1)C1=C(C1)C(C1)=C(C1)C=C1C1	XGQBSVVY
DTXSID9074222	74472-33-6	2,3,3',6-Tetrachlorobiphenyl	2,3,3',6-Tetrachloro-1,1'-biphenyl	C12H6Cl4	289.92236	291.98001	C1C1=CC=CC(=C1)C1=C(C1)C(C1)=CC=C1C1	WZNAMGY
DTXSID9074220	74338-23-1	2,3',5',6-Tetrachlorobiphenyl	2,3',5',6-Tetrachloro-1,1'-biphenyl	C12H6Cl4	289.92236	291.98001	C1C1=CC(=CC(C1)=C1)C1=C(C1)C=CC=C1C1	HDULUCZR
DTXSID9074199	68194-11-6	2,3,4',5,6-Pentachlorobiphenyl	2,3,4',5,6-Pentachloro-1,1'-biphenyl	C12H5Cl5	323.88339	326.42001	C1C1=CC=C(C=C1)C1=C(C1)C(C1)=CC(C1)=C1C1	ZDDZPDTV
DTXSID9074197	68194-08-1	2,2',3,4',6,6'-Hexachlorobiphenyl	2,2',3,4',6,6'-Hexachloro-1,1'-biphenyl	C12H4Cl6	357.84442	360.85999	C1C1=CC(C1)=C(C(C1)=C1)C1=C(C1)C(C1)=CC=C1C1	RPPNJBZN
DTXSID9074195	68194-04-7	2,2',4,6'-Tetrachlorobiphenyl	2,2',4,6'-Tetrachloro-1,1'-biphenyl	C12H6Cl4	289.92236	291.98001	C1C1=CC=C(C(C1)=C1)C1=C(C1)C=CC=C1C1	WVHNUGR
DTXSID9074193	60233-25-2	2,2',3,4',6'-Pentachlorobiphenyl	2,2',3,4',6'-Pentachloro-1,1'-biphenyl	C12H5Cl5	323.88339	326.42001	C1C1=CC(C1)=C(C(C1)=C1)C1=C(C1)C(C1)=CC=C1	GOFFZTAP
DTXSID9074191	60145-23-5	2,2',3,4,4',5,6'-Heptachlorobiphenyl	2,2',3,4,4',5,6'-Heptachloro-1,1'-biphenyl	C12H3Cl7	391.80544	395.31	C1C1=CC(C1)=C(C(C1)=C1)C1=C(C1)C(C1)=C(C1)C(C1)=C1	RXRLRYZU
DTXSID9074149	41411-61-4	2,2',3,4,5,6-Hexachlorobiphenyl	2,2',3,4,5,6-Hexachloro-1,1'-biphenyl	C12H4Cl6	357.84442	360.85999	C1C1=C(C=C=CC=C1)C1=C(C1)C(C1)=C(C1)C(C1)=C1C1	RUEIBQJF
DTXSID9074147	40186-70-7	2,2',3,3',4,4',5,6'-Heptachlorobiphenyl	2,2',3,3',4,4',5,6'-Heptachloro-1,1'-biphenyl	C12H3Cl7	391.80544	395.31	C1C1=CC(C1)=C(C1)C(=C1)C1=C(C1)C(C1)=C(C1)C=C1C1	KJBDZJFS
DTXSID9074145	39635-33-1	3,3',4,5,5'-Pentachlorobiphenyl	3,3',4,5,5'-Pentachloro-1,1'-biphenyl	C12H5Cl5	323.88339	326.42001	C1C1=CC(=CC(C1)=C1)C1=CC(C1)=C(C1)C(C1)=C1	MXVAYAXI
DTXSID9074143	38444-76-7	2,3',6-Trichlorobiphenyl	2,3',6-Trichloro-1,1'-biphenyl	C12H7Cl3	255.96133	257.54001	C1C1=CC=CC(=C1)C1=C(C1)C=CC=C1C1	VQOFJPFY
DTXSID9074141	38380-05-1	2,2',3,3',4,6'-Hexachlorobiphenyl	2,2',3,3',4,6'-Hexachloro-1,1'-biphenyl	C12H4Cl6	357.84442	360.85999	C1C1=CC=C(C1)C(=C1)C1=C(C1)C(C1)=C(C1)C=C1	OKBJVIVE
DTXSID9073599	65510-45-4	2,2',3,4,4'-Pentachlorobiphenyl	2,2',3,4,4'-Pentachloro-1,1'-biphenyl	C12H5Cl5	323.88339	326.42001	C1C1=CC(C1)=C(C=C1)C1=C(C1)C(C1)=C(C1)C=C1	LACXVZHA
DTXSID9073541	52744-13-5	2,2',3,3',5,6'-Hexachlorobiphenyl	2,2',3,3',5,6'-Hexachloro-1,1'-biphenyl	C12H4Cl6	357.84442	360.85999	C1C1=CC(=C(C1)C(C1)=C1)C1=C(C1)C(C1)=CC=C1C1	UUTNFLRS
DTXSID9073410	16606-02-3	2,4',5-Trichlorobiphenyl	2,4',5-Trichloro-1,1'-biphenyl	C12H7Cl3	255.96133	257.54001	C1C1=CC=C(C=C1)C1=C(C1)C=CC(C1)=C1	VAHKBZSA
DTXSID80873557	36559-22-5	2,2',3,4'-Tetrachlorobiphenyl	1,12,2',3,4'-Tetrachloro-1,1'-biphenyl	C12H6Cl4	289.92236	291.98	C1C1=CC(C1)=C(C=C1)C1=CC=CC(C1)=C1C1	ALFHIHQ
DTXSID8074780	61798-70-7	PCB 131	2,2',3,3',4,6-Hexachlorobiphenyl	C12H4Cl6	357.84442	360.85999	C1C1=CC(C1)=C(C1)C(C1)=C1C1=CC=CC(C1)=C1C1	WDLTVN
DTXSID8074239	74472-51-8	2,3,3',4,5,5',6-Heptachlorobiphenyl	2,3,3',4,5,5',6-Heptachloro-1,1'-biphenyl	C12H3Cl7	391.80544	395.31	C1C1=CC(=CC(C1)=C1)C1=C(C1)C(C1)=C(C1)C(C1)=C1C1	ZUTDUGM
DTXSID8074237	74472-49-4	2,2',3,4,5,6,6'-Heptachlorobiphenyl	2,2',3,4,5,6,6'-Heptachloro-1,1'-biphenyl	C12H3Cl7	391.80544	395.31	C1C1=CC=CC(C1)=C1C1=C(C1)C(C1)=C(C1)C(C1)=C1C1	FGDPOTM
DTXSID8074235	74472-47-2	2,2',3,4,4',5,6-Heptachlorobiphenyl	2,2',3,4,4',5,6-Heptachloro-1,1'-biphenyl	C12H3Cl7	391.80544	395.31	C1C1=CC(C1)=C(C=C1)C1=C(C1)C(C1)=C(C1)C(C1)=C1C1	DJEUXBQA
DTXSID8074233	74472-44-9	2,3,3',4',5,6-Hexachlorobiphenyl	2,3,3',4',5,6-Hexachloro-1,1'-biphenyl	C12H4Cl6	357.84442	360.85999	C1C1=CC=C(C=C1)C1=C(C1)C(C1)=CC(C1)=C1C1	ZAGRQXMA

How Did We Do This? DSSTox

ACToR-DSSTox Chemical Registration

View/Edit a
Single Record

Structure
Search

Browse/Curate
Records

Export DSSTox

Chemotypes

Manage
Chemical Lists

Manage
Property Data

Add Deleted
Casrns

Welcome, antony

Logout

Substance_ID: DTXSID5024267

CAS:

Name:

Substance Type:

QC Level:

Data Source:

QC Notes:

Compound_ID:

Chemical Shown:

Private Notes:

Source of CAS-Compound:

Double Stereo:

Chiral Stereo:

Chemical Form:

▶ Synonyms (31)

▶ Other Cas (0)

▼ Successor Substances (209)

	CAS-RN	Relationship	Source	Struct	Casrn	Comments
	<input type="text" value="32774-16-6"/>	is a Representative Isomer of this	<input type="text" value="STN(DSSTox)"/>	<input checked="" type="checkbox"/>	<input type="checkbox"/>	<input type="text" value="structure shown 3,3',4,4',5,5'"/>
	<input type="text" value="2051-60-7"/>	is a Representative Isomer of this	<input type="text" value="Public"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="text"/>
	<input type="text" value="2051-61-8"/>	is a Representative Isomer of this	<input type="text" value="Public"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="text"/>
	<input type="text" value="2051-62-9"/>	is a Representative Isomer of this	<input type="text" value="Public"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="text"/>
	<input type="text" value="13029-08-8"/>	is a Representative Isomer of this	<input type="text" value="Public"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="text"/>
	<input type="text" value="16605-91-7"/>	is a Representative Isomer of this	<input type="text" value="Public"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="text"/>
	<input type="text" value="25569-80-6"/>	is a Representative Isomer of this	<input type="text" value="Public"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="text"/>
	<input type="text" value="33284-50-3"/>	is a Representative Isomer of this	<input type="text" value="Public"/>	<input type="checkbox"/>	<input type="checkbox"/>	<input type="text"/>

- Various relationship mappings can be established. To this point all are manual.

Relationship	Source
is a Representative Isomer of this	STN(DSSTox) ▼
is a Representative Component of this substance	
is a Mixture Component of this substance	
is a Monomer of this substance	
is an Active Ingredient of this substance	
is a Representative Isomer of this substance	
is a General Form of this substance	
is a Transformation Product of this substance	

- In progress – **metabolite** mappings (building metabolism competence into high-throughput assay)

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TSCA Chemical Substance Inventory

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- TSCA Inventory Home
- About the Inventory
- Access the Inventory
- Policy and Guidance

Chemical Substances of Unknown or Variable Composition, Complex Reaction Products and Biological Materials (UVCB Substance) on the TSCA Inventory

This paper is a compendium of information related to the broad class of chemical substances referred to as UVCBs for the Toxic Substances Control Act (TSCA) Chemical Substance Inventory. These chemical substances cannot be represented by unique structures and molecular formulas.

- UVCB chemical examples
 - Surfactants with undefined composition
 - Petroleum Distillates
 - Gelatins, hydrozylates
 - Formaldehyde, reaction products with diethanolamine
 - Fatty acids, linseed-oil, compds. with triethylamine

Managing UVCB Relationships

Alkylbenzenesulfonate, linear

42615-29-2 | DTXSID3020041

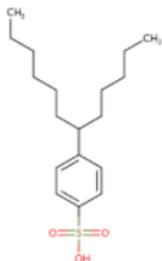
i Searched by Synonym: Found 1 result for
'Linear alkylbenzene sulfonate'.

Presence in Lists

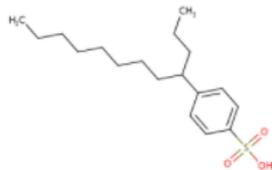
Surfactant List Screened in Swiss Wastewater (2014)

Surfactant List Screened in Swiss Wastewater (2014)

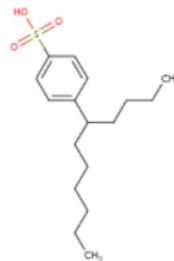
EAWAGSURF is a list of surfactants screened in Swiss wastewater effluents as part of a 2014 study. Structures/mixtures are being progressively curated and linked (Schymanski/Williams). Further details in Schymanski et al 2014, DOI: 10.1021/es4044374



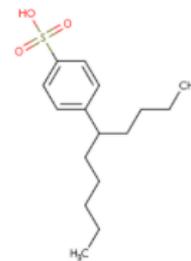
4-(Dodecan-6-yl)benzene-1-sulfon...
23003-92-1



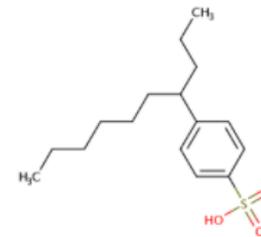
4-(dodecan-4-yl)benzene-1-sulfoni...
NOCAS_862870



C11-LAS
NOCAS_881097



4-(decan-5-yl)benzene-1-sulfonic ...
NOCAS_881146



4-(decan-4-yl)benzenesulfonic acid
NOCAS_891333

Toxicity ForeCaster (ToxCast™) Data

EPA's most updated, publicly available high-throughput toxicity data on thousands of chemicals. This data is generated through the EPA's ToxCast research effort. ToxCast is part of the Toxicology in the 21st Century (Tox21) federal collaboration. All data is available for download and includes the following data sets. The release date and version names for the data sets are provided in the table below.

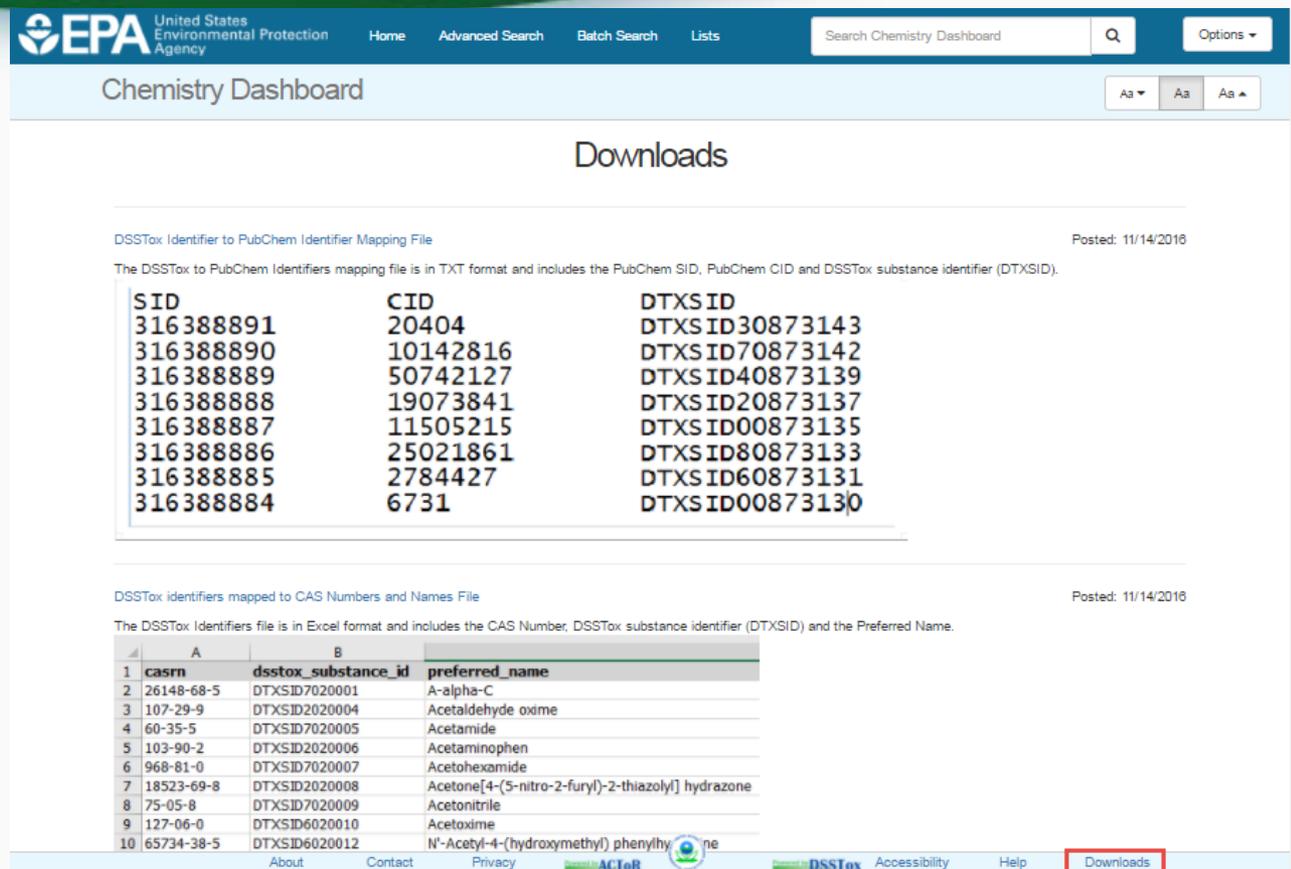
As part of EPA's commitment to share data, all of the computational toxicology data is publicly available for anyone to access and use. EPA's computational toxicology data is considered "open data", and thus all of the data below are free of all copyright restrictions, and fully and freely available for both non-commercial and commercial use.



- **ToxCast & Tox21 Chemicals:** A list of all chemicals screened, along with descriptions.
- **ToxCast & Tox21 High-throughput Assays:** Information about the hundreds of assays used to screen the chemicals.
- **ToxCast & Tox21 Summary Data:** Summary hit calls for all chemicals and concentration response curves for all assays.
- **MySQL Database:** Downloadable database that provides access to EPA's analysis of the ToxCast and Tox21 high-throughput screening data.
- **R Package:** The computer programming package used to process and model all EPA ToxCast and Tox21 chemical screening data.
- **Data Spreadsheet:** Spreadsheet that provides access to EPA's analysis of the ToxCast and Tox21 high-throughput screening data.
- **Concentration Response Curves:** Concentration response curves for all ToxCast & Tox21 assays.
- **Collaborative Estrogen Receptor Activity Prediction Project Data:** Data and supplemental files from CERAPP, a large-scale modeling project.

<https://www.epa.gov/chemical-research/toxicity-forecaster-toxcasttm-data>

Delivering our Chemistry Data



The screenshot shows the EPA Chemistry Dashboard interface. At the top, there is a navigation bar with the EPA logo, "United States Environmental Protection Agency", and links for "Home", "Advanced Search", "Batch Search", and "Lists". A search bar labeled "Search Chemistry Dashboard" and an "Options" dropdown are also present. Below the navigation bar, the page title "Chemistry Dashboard" is displayed. The main content area is titled "Downloads" and features two download links:

- DSSTox Identifier to PubChem Identifier Mapping File** (Posted: 11/14/2016)
The DSSTox to PubChem Identifiers mapping file is in TXT format and includes the PubChem SID, PubChem CID and DSSTox substance identifier (DTXSID).

SID	CID	DTXS ID
316388891	20404	DTXS ID30873143
316388890	10142816	DTXS ID70873142
316388889	50742127	DTXS ID40873139
316388888	19073841	DTXS ID20873137
316388887	11505215	DTXS ID00873135
316388886	25021861	DTXS ID80873133
316388885	2784427	DTXS ID60873131
316388884	6731	DTXS ID00873130

- DSSTox identifiers mapped to CAS Numbers and Names File** (Posted: 11/14/2016)
The DSSTox Identifiers file is in Excel format and includes the CAS Number, DSSTox substance identifier (DTXSID) and the Preferred Name.

	A	B	
1	casn	dsstox_substance_id	preferred_name
2	26148-68-5	DTXSID7020001	A-alpha-C
3	107-29-9	DTXSID2020004	Acetaldehyde oxime
4	60-35-5	DTXSID7020005	Acetamide
5	103-90-2	DTXSID2020006	Acetaminophen
6	968-81-0	DTXSID7020007	Acetohexamide
7	18523-69-8	DTXSID2020008	Acetone[4-(5-nitro-2-furyl)-2-thiazolyl] hydrazone
8	75-05-8	DTXSID7020009	Acetonitrile
9	127-06-0	DTXSID6020010	Acetoxime
10	65734-38-5	DTXSID6020012	N'-Acetyl-4-(hydroxymethyl) phenylhydrazone

At the bottom of the page, there is a footer with links for "About", "Contact", "Privacy", "ACToR", "DSSTox", "Accessibility", "Help", and "Downloads". The "Downloads" link is highlighted with a red box.

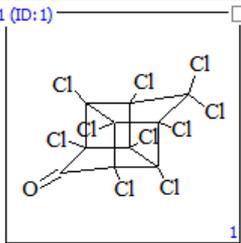
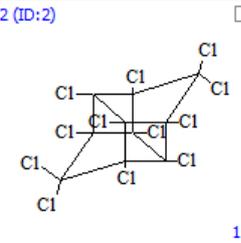
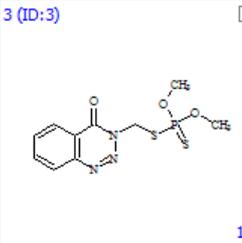
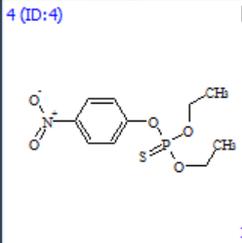
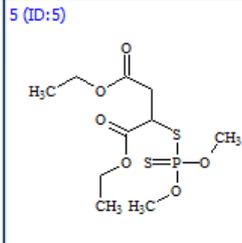
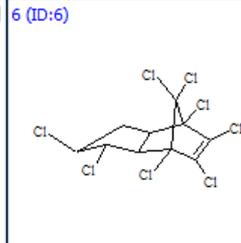
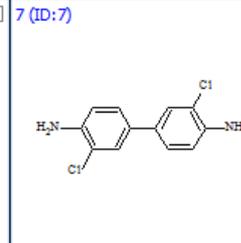
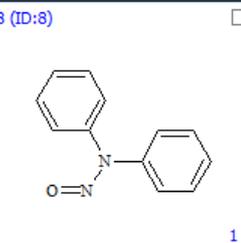
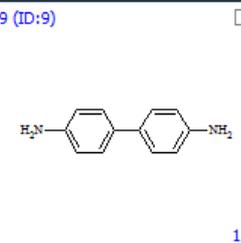
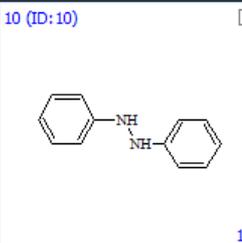
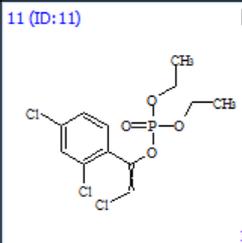
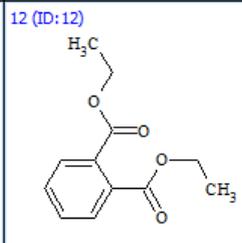
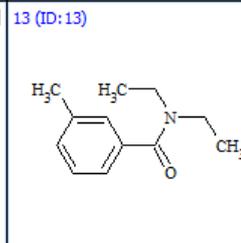
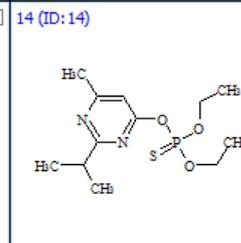
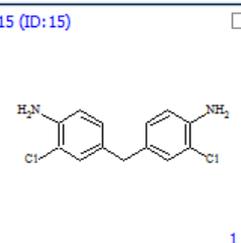
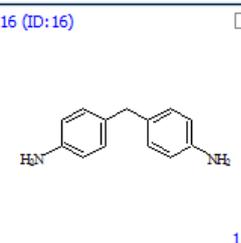
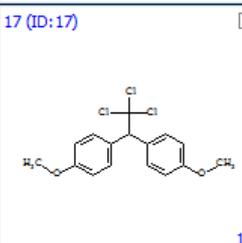
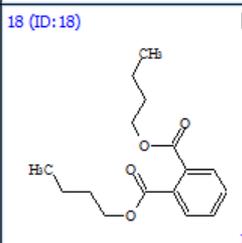
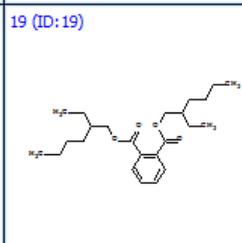
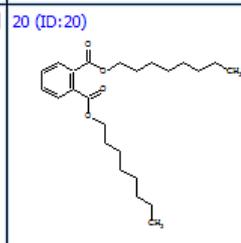
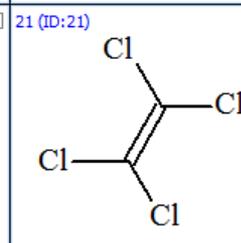
- Various types of data at FTP download site:
ftp://newftp.epa.gov/COMPTOX/Sustainable_Chemistry_Data/Chemistry_Dashboard

SDF Download

ACD/Spectrus DB: Database Window - [C:\USERS\AW...OWNLOADS\CHEMISTRYDASHBOARD-ADVANCEDSEARCH_2017-08-14_12-14-55.SDF]

Database View Record Search Lists Plates Options ACD/Labs Help



1 (ID:1)  1	2 (ID:2)  1	3 (ID:3)  1	4 (ID:4)  1	5 (ID:5)  1	6 (ID:6)  1	7 (ID:7)  1
8 (ID:8)  1	9 (ID:9)  1	10 (ID:10)  1	11 (ID:11)  1	12 (ID:12)  1	13 (ID:13)  1	14 (ID:14)  1
15 (ID:15)  1	16 (ID:16)  1	17 (ID:17)  1	18 (ID:18)  1	19 (ID:19)  1	20 (ID:20)  1	21 (ID:21)  1

ID: 1 A: 1/89 B: 89 Last Updated: 14/08/2017 12:16 Single DB

1-ChemSketch 2-Database 3-Processor

Open Data Reuse on iOS

CompTox Mobile

View in iTunes

This app is designed for both iPhone and iPad

Free

Category: Productivity
Released: Jan 16, 2017
Version: 1.0
Size: 267 MB
Language: English
Seller: Kirill Blinov
© 2017 Molecule Apps,
2017 EPA
Rated 4+

Compatibility: Requires iOS 6.0 or later. Compatible with iPhone, iPad, and iPod touch.

Customer Ratings

We have not received enough ratings to display an average for the current version of this application.

More by Kirill Blinov



NMR

View in Mac App Store

Description

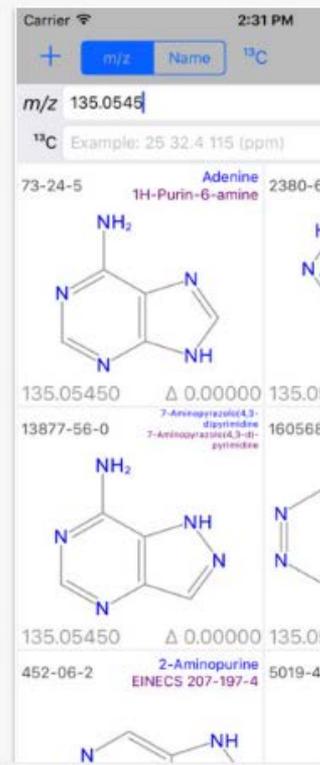
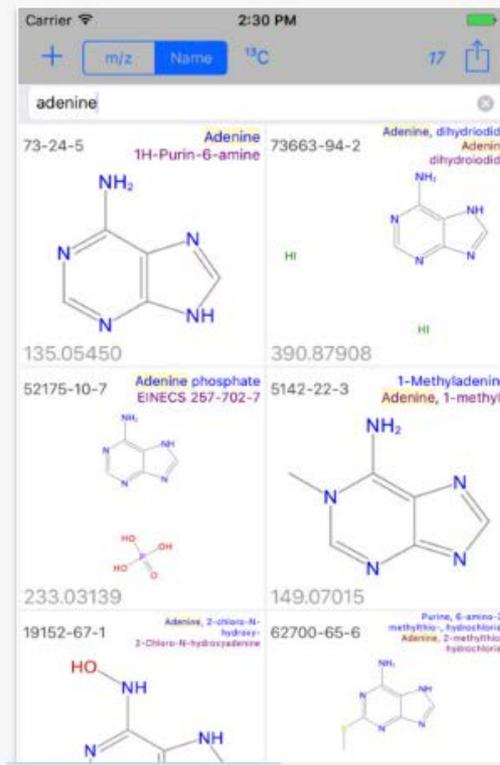
Find chemical structure instantly by exact mass (m/z), ¹³C NMR chemical shifts, structure name or CAS Registry Number in a database of about 720,000 EPA CompTox structures.

[Kirill Blinov Web Site](#) [CompTox Mobile Support](#)

...More

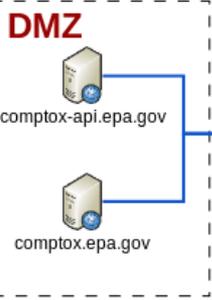
Screenshots

iPhone | iPad



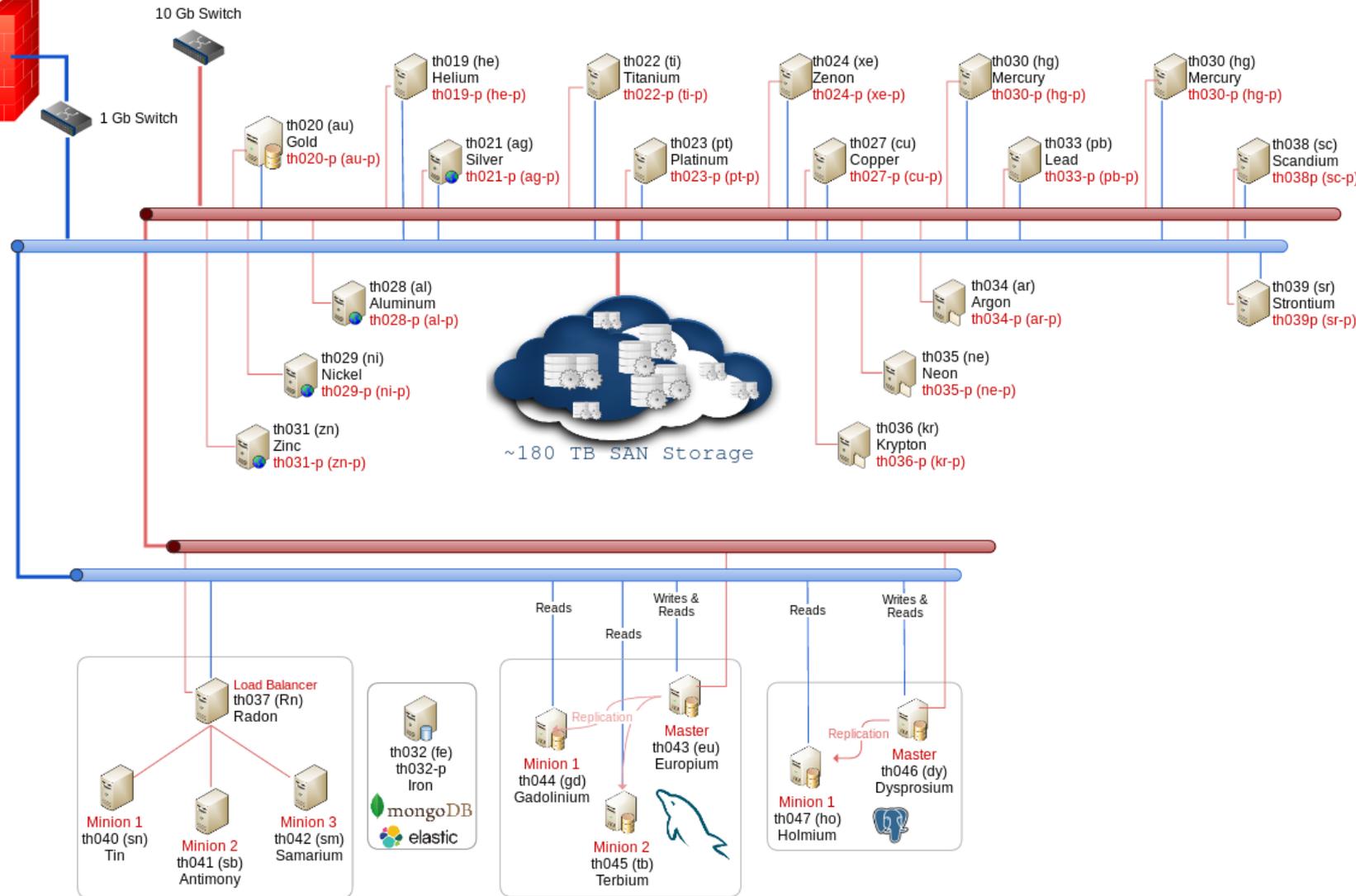
- 10 years of development – heterogeneous
 - MySQL, Java, R-code, Matlab, multiple Javascript environments, 100s of web services
 - Multiple projects, loose connectivity
- Migration to homogeneity for production Apps
 - MySQL
 - Java
 - JQuery/JavaScript
 - Versioned microservices
- Sprint methodology with Atlassian management tools
 - **Confluence** – knowledge management
 - **Jira** – ticketing/stories (work assignments)
 - **Fisheye** – collaborative peer code review
 - **Bitbucket** – code version control system

Computational Infrastructure

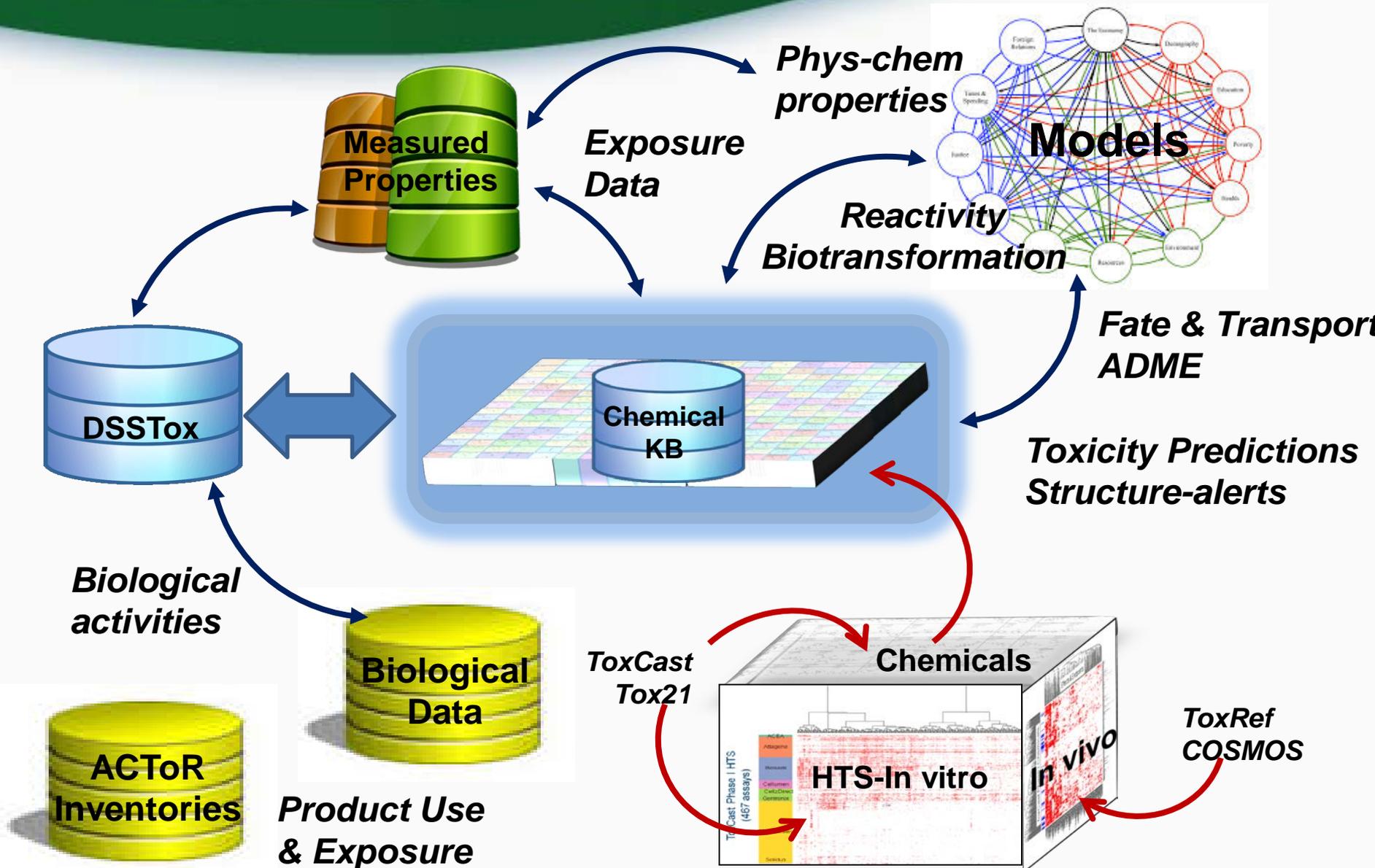


Conceptual Infrastructure

2016-11-17



We're not done yet...



OPERA Services in development

```
{
  "meta": {
    "statusCode": 200,
    "status": "success",          // [success | fail | error]
    "success": true,             // [true | false]
    "message": "string",        // A specific informational message...
    "warnings": "string",       // A warning message like: "LEADING ZEROS STRIPPED"
    "selfUrl": "http://api.zn.epa.gov/dsstox/chemicals", // The URL for THIS resource.
  },
  "data": [{
    "dsstox_cid": "DTXCID101",
    "inchi": "InChI=1S/C11H9N3/c12-10-6-5-8-7-3-1-2-4-9(7)13-11(8)14-10/h1-6H,(H3,12,13,14)",
    "inchiKey": "FJTNLJLPLJDTRM-UHFFFAOYSA-N",
    "model_name": "OPERA_LogP",
    "model_version": "v1.1.4",
    "predicted_property_id": 45433098
    "predicted_value": 2.53385
    "global_ad": 1
    "local_ad": 0.865944
    "confidence_score": 0.618723
  }],
}
```

T.E.S.T services (ALPHA)

← ⓘ 🔒 [https://comptox.epa.gov/dashboard/web-test/WS?smiles=C1C\(Cl\)\(Cl\)Cl](https://comptox.epa.gov/dashboard/web-test/WS?smiles=C1C(Cl)(Cl)Cl)

JSON Raw Data Headers

Save Copy

```
uuid: "919325ac-14e5-45b5-b932-e401b79edf8c"
predictionTime: 1502741333903
software: "T.E.S.T (Toxicity Estimation Software Tool)"
softwareVersion: "4.2"
condition: "25°C"
endpoint: "Water solubility at 25°C"
method: "Consensus"
▼ predictions:
  ▼ 0:
    id: "C_1502741333903"
    smiles: "C1C(Cl)(Cl)Cl"
    expVal: "2.288"
    expValMass: "792.473"
    predVal: "2.186"
    predValMass: "1003.411"
```

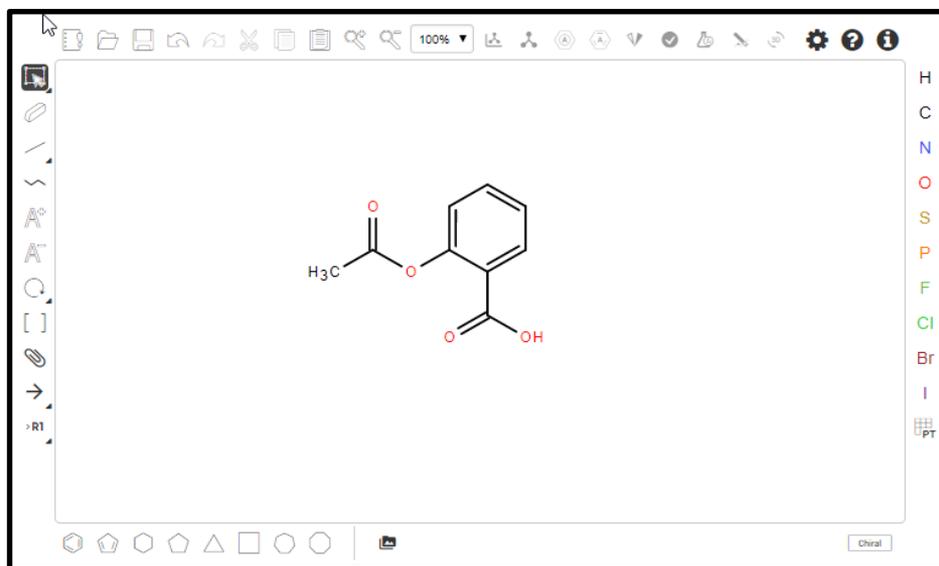
T.E.S.T services (ALPHA)

- 96hr fathead minnow 50% lethal concentration (LC50)
- 48hr daphnia magna 50% lethal concentration (LC50)
- Tetrahymena pyriformis 50% growth inhibition conc. (IGC50)
- Oral rat 50% lethal dose (LD50)
- Bioconcentration Factor (BCF)
- Developmental Toxicity (DevTox)
- Ames Mutagenicity (Mutagenicity)
- Normal boiling point, Flash point, Melting point
- Surface tension, Viscosity, Water Solubility
- Thermal Conductivity, Vapor Pressure, Density

Real time predictions

Chemistry Dashboard

Search a chemical by systematic name, synonym, CAS number, or InChIKey



Select properties to predict

T.E.S.T. 18 OPERA EPI Suite

- TOXICITY** + -
 - Fathead minnow LC50 (96 hr) ⓘ
 - Daphnia magna LC50 (48 hr) ⓘ
 - T. pyriformis IGC50 (48 hr)
 - Oral rat LD50
 - Bioaccumulation factor
 - Estrogen Receptor RBA
- ACTIVITY** + -
 - Developmental Toxicity
 - Mutagenicity
 - Estrogen Receptor Binding
- PHYS_CHEM** + -
 - Normal boiling point
 - Vapor pressure at 25°C
 - Melting point
 - Flash point
 - Density
 - Surface tension at 25°C

Calculate

Real time predictions

Chemistry Dashboard

Provider: TEST

Download table as:

Property	Experimental Value	Prediction				
		Consensus	Hierarchical clustering	Single model	Group contribution	Nearest neighbor
Fathead minnow LC50 (96 hr)		3.309 Log10(mol/L) 88.471 mg/L	3.286 Log10(mol/L) 93.341 mg/L	2.901 Log10(mol/L) 226.071 mg/L	3.240 Log10(mol/L) 103.561 mg/L	3.808 Log10(mol/L) 28.034 mg/L
Daphnia magna LC50 (48 hr)		3.271 Log10(mol/L) 96.599 mg/L	3.956 Log10(mol/L) 19.942 mg/L	3.858 Log10(mol/L) 24.999 mg/L	1.998 Log10(mol/L) 1808.159 mg/L	
T. pyriformis IGCS0 (48 hr)		2.411 Log10(mol/L) 698.990 mg/L			1.982 Log10(mol/L) 1876.118 mg/L	2.840 Log10(mol/L) 260.425 mg/L
Oral rat LD50	2.955 Log10(mol/kg) 199.840 mg/kg	2.637 Log10(mol/kg) 415.666 mg/kg	2.942 Log10(mol/kg) 206.130 mg/kg			2.332 Log10(mol/kg) 838.203 mg/kg
Bioaccumulation factor		0.031 Log10 1.073	0.166 Log10 1.465	-0.161 Log10 0.690	-0.242 Log10 0.572	0.361 Log10 2.295
Estrogen Receptor RBA						-3.293 Log10 5.089*10 ⁻⁴
Developmental Toxicity		true	true	true		
Mutagenicity						

DEVELOPMENT

- Continuous updating of lists and ongoing curation
- Integration to other agency databases – ECOTOX, ChemView
- Structure and substructure searching in development
- Release of Analytical QC data for ToxCast
- Further Non-Targeted Analysis support – spectral search
- Open API and web services
- “CompTox ~~Chemistry~~ Dashboard” will integrate other dashboards over time (i.e. EDSP21 and ToxCast)

Acknowledgements



Credit: the Research Triangle Foundation

EPA-RTP

*An enormous team of
contributors from NCCT*

and collaborators from

NERL

NHERL

NRMRL

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>