

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

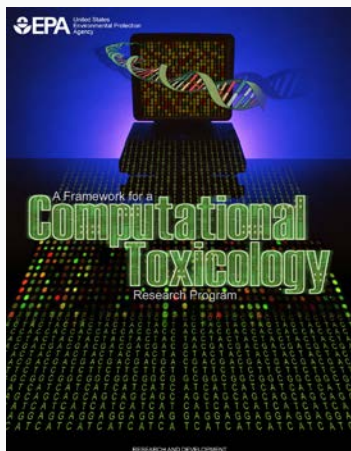
Antony Williams

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.

*NORMAN Network-UFZ
30th 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)

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.

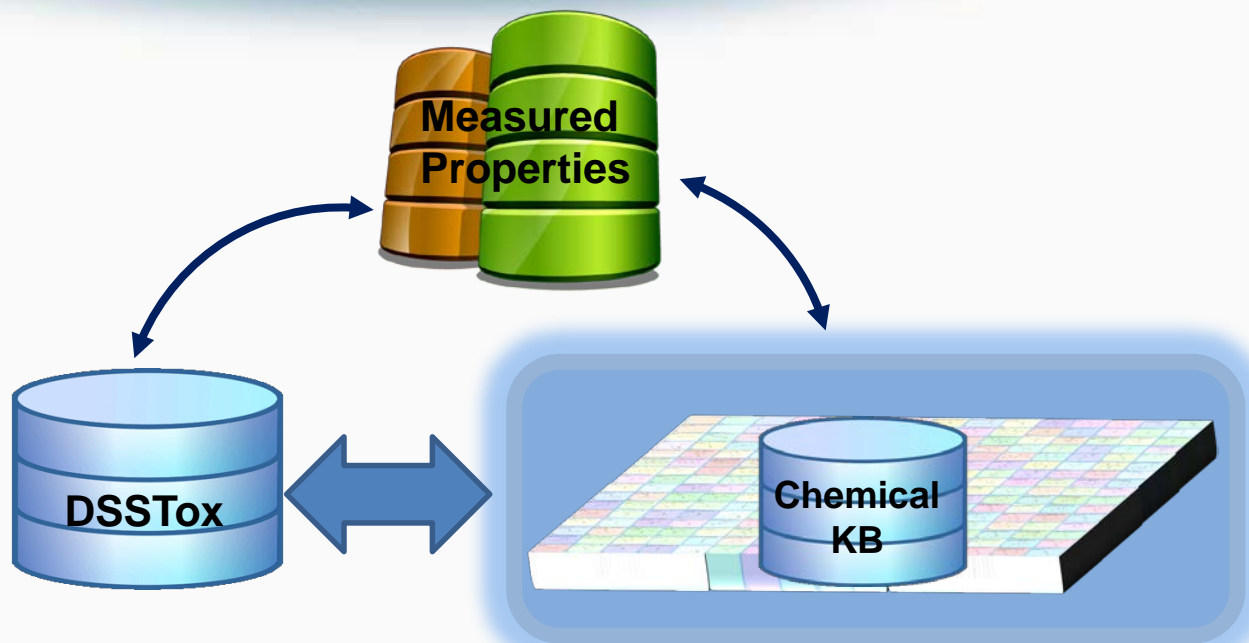
- [ToxCast Data](#): High-throughput screening data on thousands of chemicals.

Rapid Exposure and Dose Data

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

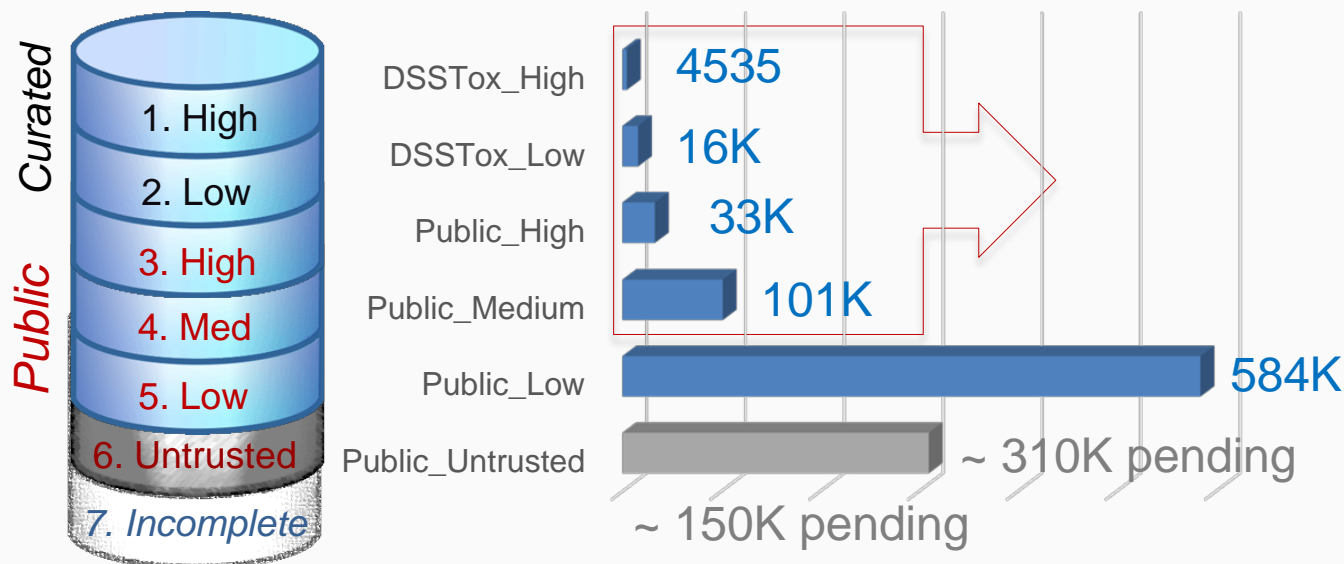
- [High-throughput toxicokinetics data](#): It is important to link the external dose of a chemical to an internal blood or tissue concentration. This process is called toxicokinetics. EPA researchers measure the critical factors that determine the distribution

Underpinning with chemicals



Approximately 17 Years of Data...

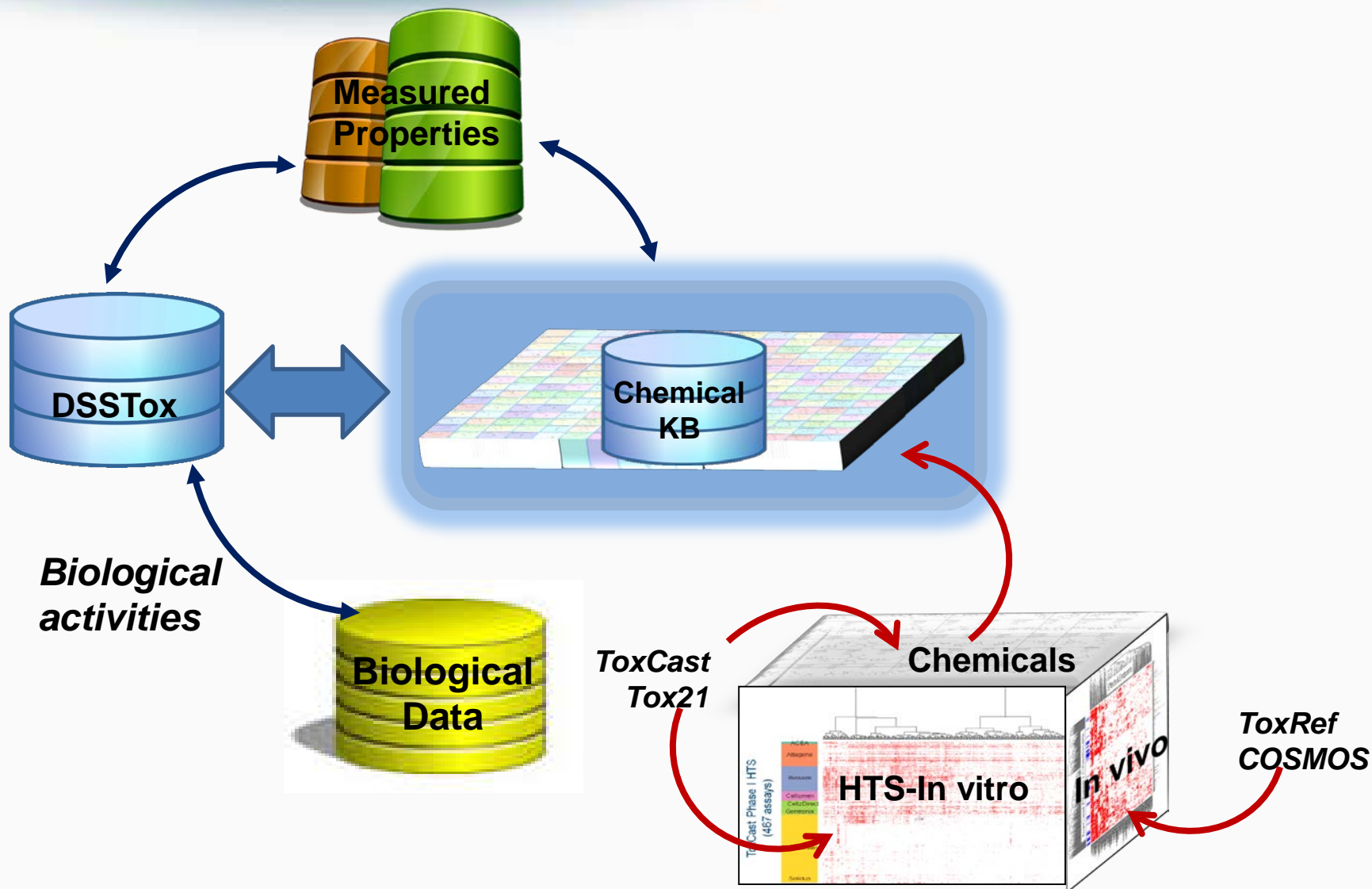
Growing with daily curation








QC Levels

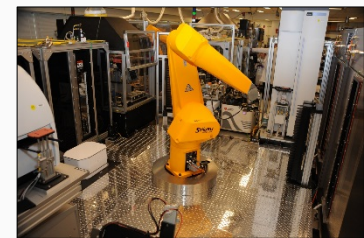
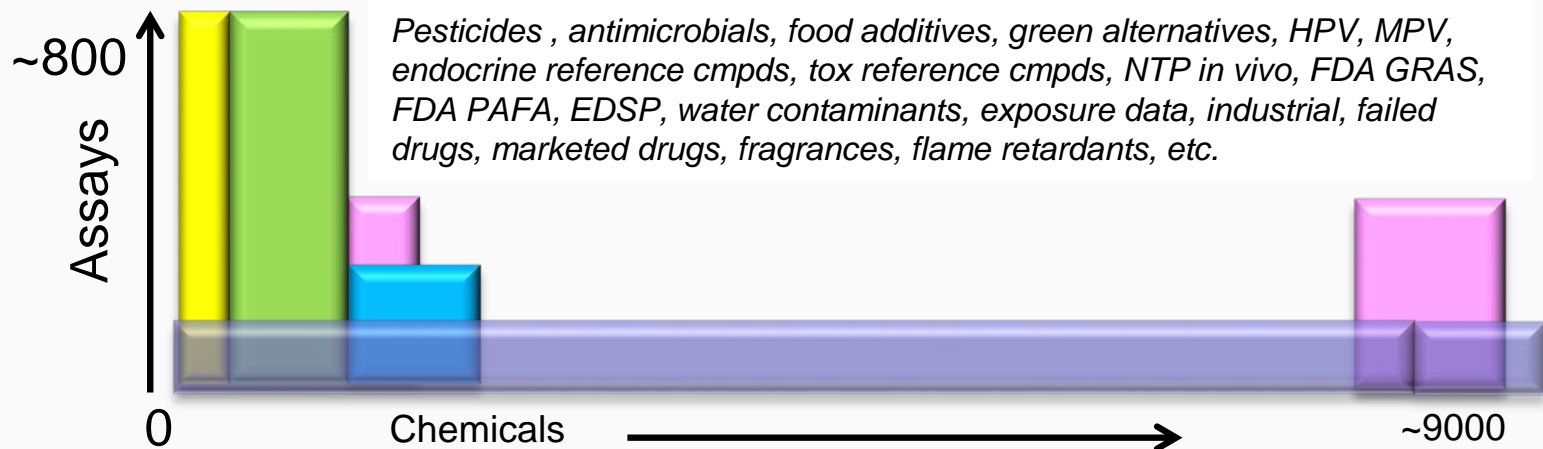
DSSTox_High:	Hand curated and validated
DSSTox_Low:	Hand curated and confirmed using multiple public sources
Public_High:	Extracted from EPA SRS and confirmed to have no conflicts in ChemID and PubChem
Public_Medium:	Extracted from ChemID and confirmed to have no conflicts in PubChem
Public_Low:	Extracted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

Integrating *in vitro* and *in vivo* data

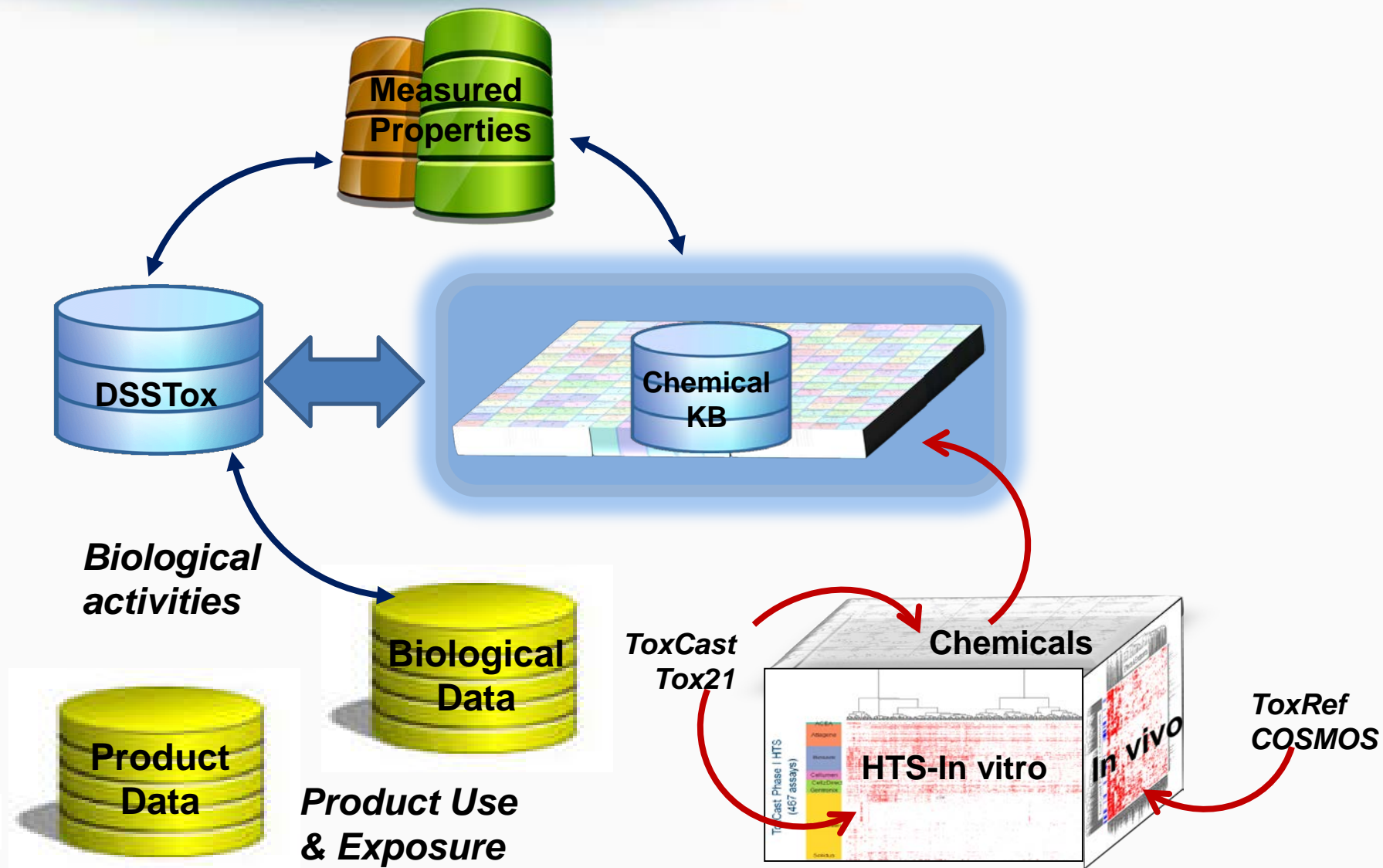


TEN YEARS of Assay Measurements: ToxCast & Tox21

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

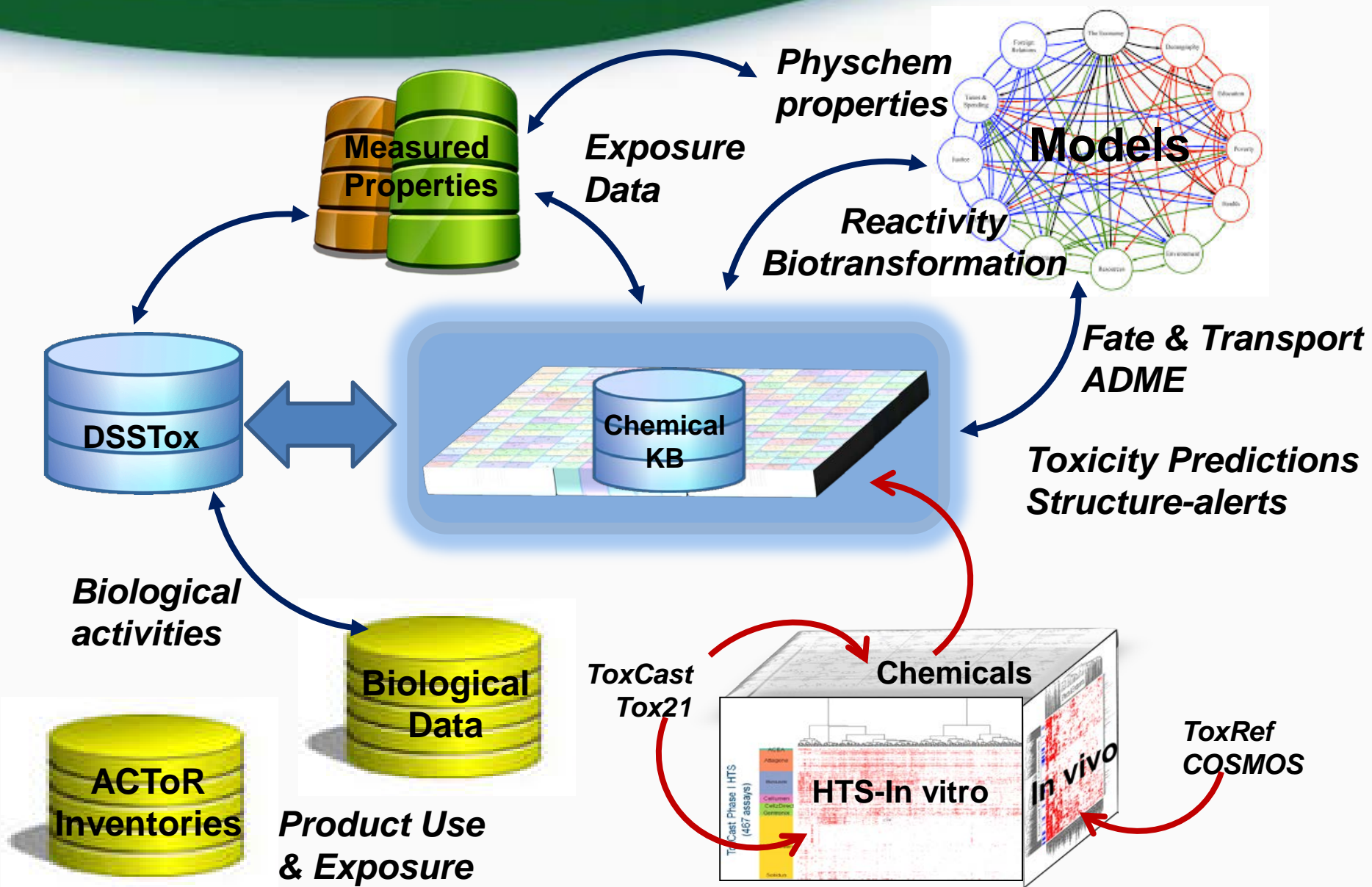
EPA is currently evaluating the effectiveness of high throughput exposure models



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
- We are building: CompTox Chemistry Dashboard


Comptox Chemistry Dashboard

<https://comptox.epa.gov>


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Environmental Protection
Agency

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Chemistry Dashboard As ▼ As As ▲



Chemistry Dashboard





☐ Single component search ☐ Ignore isotopes

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~760,000 chemicals
>17 years of data


Comptox Chemistry Dashboard

<https://comptox.epa.gov>


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Home Advanced Search Batch Search Lists



Chemistry Dashboard As ▼ As As ▲

 UNITED STATES
ENVIRONMENTAL PROTECTION AGENCY

Chemistry Dashboard



- 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)

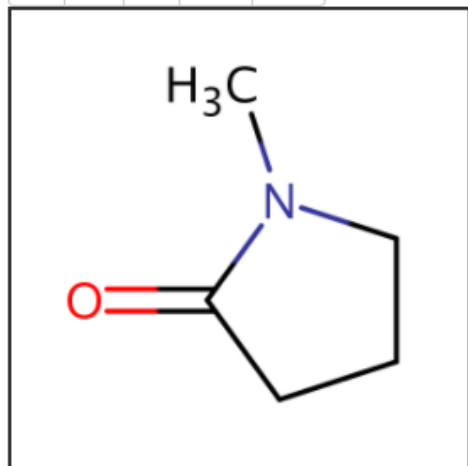
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~760,000 chemicals
>17 years of data

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

Average Mass: 99.133 g/mol

Monoisotopic Mass: 99.068414 g/mol

[Find All Chemicals](#)



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

LogK_{ow}: 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 ² 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
LogK _{ow} : 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	100.12 (1)	100.12 (1)	100.12	100.12	100.12	100.12	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

- Our approach to modeling:
 - Obtain **high quality** training sets
 - Apply appropriate modeling approaches
 - **Validate** performance of models
 - Define the applicability domain and model limitations
 - Use models to predict properties across our full datasets
 - Release as **Open Data and Open Models**

Multiple Prediction Algorithms Transparency is Important

Summary	LogP: Octanol-Water			
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

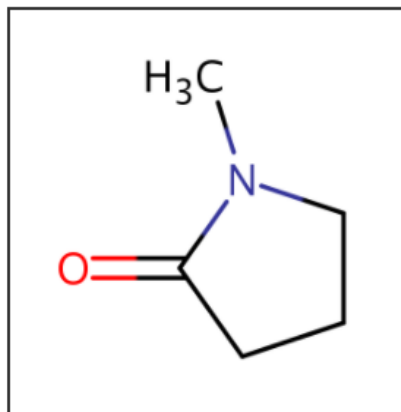
Download as: [TSV](#) [Excel](#) [SDF](#)

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

N-Methyl-2-pyrrolidone

872-50-4 | DTXSID6020856



Model Results

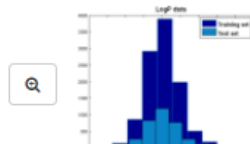
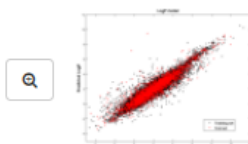
Predicted value: -0.300

Global applicability domain: **Inside** ⓘ

Local applicability domain index: 0.88 ⓘ

Confidence level: 0.81 ⓘ

Model Performance



Weighted KNN model

QMRf

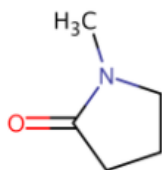
5-fold CV (75%)

Training (75%)

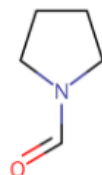
Test (25%)

Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.88	0.67	0.88	0.78

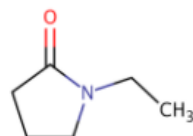
Nearest Neighbors from the Training Set



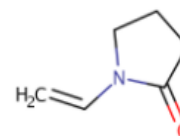
N-Methyl-2-pyrrolidone
Measured: -0.380
Predicted: -0.300



Prolinal
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]


Customize [Icon]

1 / 11 [Navigation Icons] 125% [Zoom]

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 QMRF
 - 2.2.QMRF author(s) and contact details
 - 2.3.Date of QMRF update(s)
 - 2.4.QMRF 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 QMRF 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



QMRF identifier (JRC Inventory): To be entered by JRC
QMRF 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



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

Enter keywords, authors, DOI etc.

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

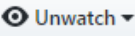


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
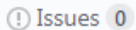

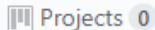


 <http://dx.doi.org/10.1080/1062936X.2016.1253611>

 Check for updates

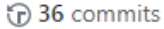
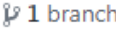



OPERA on GitHub

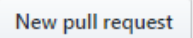
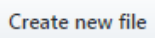
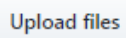


 This repository Search Pull requests Issues Marketplace Gist   


kmansouri / OPERA  1  1  0

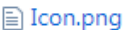
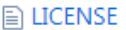

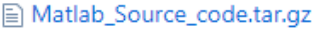
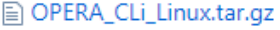


 Code  Issues 0  Pull requests 0  Projects 0  Wiki  Insights

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>

Toxicity Values

Bioavailability Metric

Download as:

TSV

Excel

Exposure Limit

Point Of Departure

Regulatory Toxicity Value

Effect Level

Misc Hazard Information

Screening Level

Uncertainty Factor

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

Product Composition Details


Product & Use Categor...

Chemical Weight Fra...

Chemical Functional Use

Monitoring Data

Exposure Predictions

Chemical Weight Fractions 

Download as:

TSV

Excel

<u>Product Name</u>	<u>Product Use Category</u>	<u>Minimum Weight Fraction</u>	<u>Maximum Weight Fraction</u>	<u>Data Type</u>	<u>Source</u>
10-02199- calico tip & ...	personal care: nail poli...	0.01	0.05	MSDS	Retail Product Categori...
6095-6096 minwax wo...	home maintenance: fin...	0.01	0.01	MSDS	Retail Product Categori...
6095/6096 minwax wo...	home maintenance: fin...	0.01	0.01	MSDS	Retail Product Categori...
ab artificial nail remove...	personal care: nail poli...	0.01	0.03	MSDS	Retail Product Categori...
artificial nail remover 7...	personal care: nail poli...	0.01	0.05	MSDS	Retail Product Categori...
calico tip & glue remov...	personal care: nail poli...	0.01	0.05	MSDS	Retail Product Categori...
citristrip canadian strip...	home maintenance: str...	0.65	0.7	MSDS	Retail Product Categori...
citristrip stripping gel q...	home maintenance: str...	0.4	0.55	MSDS	Retail Product Categori...
citristrip stripping gel q...	home maintenance: str...	-	-	MSDS	Retail Product Categori...

Chemical Properties

Env. Fate/Transport

Toxicity Values (Beta)

ADME (Beta)

Exposure

Bioassays

Similar Molecules (Beta)

Synonyms

Literature

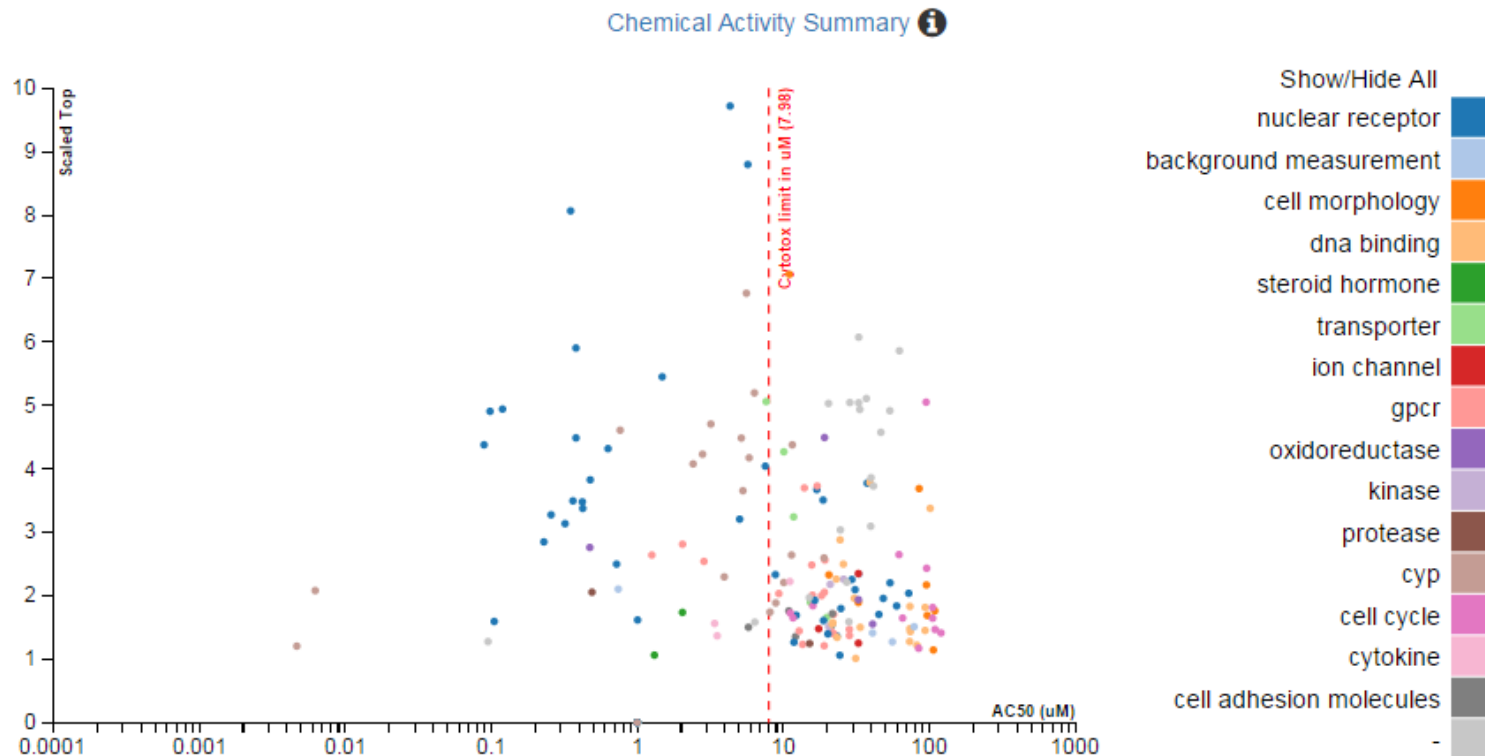
External Links

ToxCast and Tox21 Bioassays

ToxCast

PubChem

ScrubChem (Beta)



Chemical Properties

Env. Fate/Transport

Synonyms

External Links

Toxicity Values (Beta)

Exposure

Bioassays

Similar Molecules (Beta)

Literature

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

Chemical Properties

Env. Fate/Transport

Synonyms

External Links

Toxicity Values (Beta)

Exposure

Bioassays

Similar Molecules (Beta)


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

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

Case law

My library

Any time

Since 2017

Since 2016

Since 2013

Custom range...

Sort by relevance

Sort by date

☒ include patents

☒ include citations

☒ Create alert

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

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

... 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. ...

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](#)

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

CA Mullin - *Current Opinion in Insect Science*, 2015 - Elsevier

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

[Cited by 9](#) [Related articles](#) [All 2 versions](#) [Web of Science: 6](#) [Cite](#) [Save](#) [More](#)

[Biological monitoring: exquisite research probes, risk assessment, and routine exposure measurement](#)

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

ADVERTISEMENT. ...

[Cited by 19](#) [Related articles](#) [All 5 versions](#) [Web of Science: 10](#) [Cite](#) [Save](#)

[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](#)

Chemical Properties

Env. Fate/Transport

Toxicity Values (Beta)

ADME (Beta)

Exposure

Bioassays

Similar Molecules (Beta)

Synonyms

Literature

External Links

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

Chemical Properties

Env. Fate/Transport

Toxicity Values (Beta)

ADME (Beta)

Exposure

Bioassays

Similar Molecules (Beta)

Synonyms

Literature

External Links

Integrated Literature Searching

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 meas  ents to determine the source of exposure can be useful. The possibility of skin absorption from use of

Chemical Properties

Env. Fate/Transport

Toxicity Values (Beta)

ADME (Beta)

Exposure

Bioassays

Similar Molecules (Beta)














Synonyms

Literature













External Links

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...

U.S. Department of Health & Human Services www.hhs.gov

National Institutes of Health

English | Español

ChemHAT.org



ECHA
EUROPEAN CHEMICALS AGENCY

Search the ECHA Website

About Us Regulations Addressing Chemicals of Concern Information on Chemicals Chemicals in our Life Support


N-methyl-2-pyrrolidone
CAS: 872-50-4

ECHA > Substance Information


How to use Substance Information

Infocards are automatically generated for each substance.


Acute

 Irritant
Irritant to eyes.

Chronic

 Birth defects
Developmental effects on biol. app.

Other

 Other
Serious

1-methyl-2-pyrrolidone

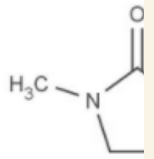
Other names: Regula

Substance identification

EC / List no.: 212

CAS no.: 872-50-4

Mol. formula: C₅H₉NO



About this substance

This substance is used by consumers, by professional workers (widespread uses), in formulation or re-

MoNA - MassBank of North America

Spectra Downloads Upload Help

Search...

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	CN1CCCC1=O
molecular formula	C ₅ H ₉ NO
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

Aa Aa Aa

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

Aa Aa Aa

NormaNEWS: Norman Early Warning System

Search NORMANEWS Chemicals

Q

List Details

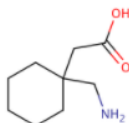
Description: The Norman Early Warning System (NormaNEWS) is a pilot network designed to investigate the spatial and temporal distribution of newly identified contaminants of emerging concern in environmental samples through performing retrospective suspect screening on HRMS data acquired using different 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

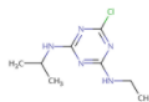
Sort Options Select/Deselect All Download as: TSV Excel SDF

View Selected

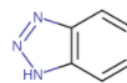
View Selected



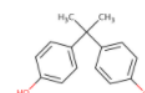
Gabapentin
60142-96-3



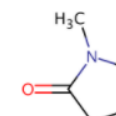
Atrazine
1912-24-9



1,2-Benzotriazole
95-14-7



Bisphenol A
80-05-7



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

About

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DSSTox


Accessibility

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Crowdsourced Curation – HELP!

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

 United States
Environmental Protection
Agency

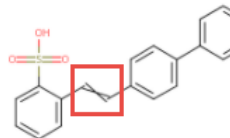
Home Advanced Search Batch Search Lists


Search All Data 

Chemistry Dashboard Submit Comment Share ▾ Copy ▾ Aa ▾ Aa Aa ▴

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

© Searched by DSSTox_Substance




New Comment 

Comment




Type your comments here...

Email address

Enter your email address

☐ I'm not a robot 
reCAPTCHA
Privacy - Terms

Submit

Find All Chemicals 



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							
<div>Add A Comment</div>								

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.

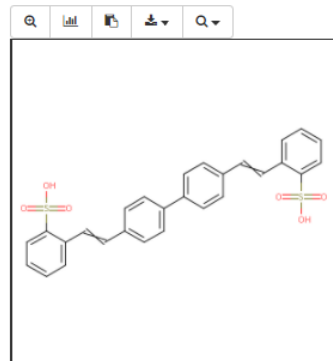
User comment posted 1 day ago

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

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'-diyl-di-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

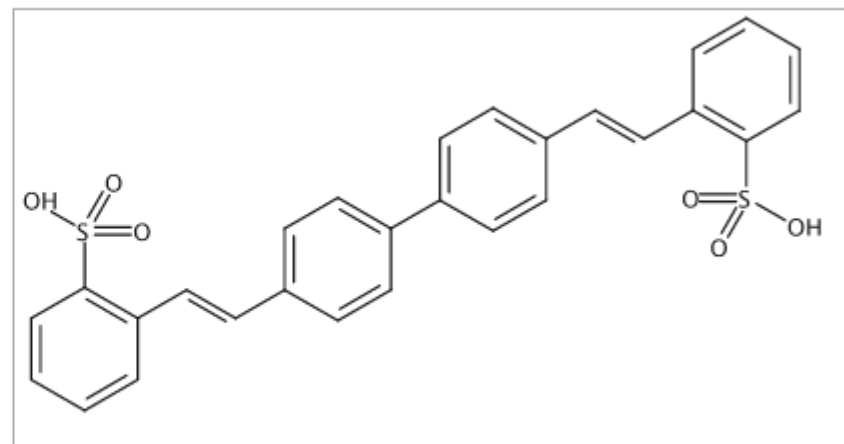
2,2'-([1,1'-Biphenyl]-4,4'-diyl-di-2,1-ethenediyl)bis[benzenesulfonic acid]

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

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


C.I. 482200

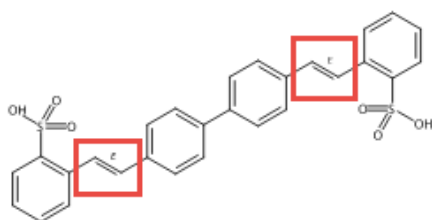
C.I. Fluorescent Brightener 351



Curation is laborious work

1. **334756-45-5** 🔍

~5  ~1 



Double bond geometry as shown.

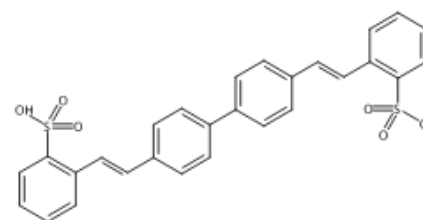
C₂₈ H₂₂ O₆ S₂

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

► **Key Physical Properties**

2. **38775-22-3** 🔍

~160  ~17 



C₂₈ H₂₂ O₆ S₂

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

► **Key Physical Properties**

Regulatory Information

Curation from YESTERDAY

NORMAN-SusDat: NORMAN Suspect List Exchange Merged Data Table

[Reset search results](#)

Show entries

Mol_ID ▲ Name CAS_RN ValidationLevel SMILES

<input type="text"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>
SA10004	garamicidin D	CAS_RN: 1405-97-6	Level 5	<chem>CC(C)C[C@@H](NC(=O)[C@H](C)NC(=O)CNC(=O)[C@@H](NC(=O)C(C)C)C(=O)N[C@@H](C)C(=O)N[C@H](C(C)C)C(=O)N[C@@H](C(C)C)C(=O)N[C@@H](Cc1c[nH]c2ccccc12)C(=O)N[C@H](CC(C)C)C(=O)N[C@@H](Cc1c[nH]c2ccccc12)C(=O)N[C@@H](CC(C)C)C(=O)N[C@@H](Cc1c[nH]c2ccccc12)C(=O)N[C@H](CC(C)C)C(=O)N[C@@H](Cc1c[nH]c2ccccc12)C(=O)NCCO</chem>

- Gramicidin D not Garamicidin D
- CASRN 1405-07-6

1. 1405-97-6

~1774



~23



Substance
Image
Cannot Be
Displayed
1405-97-6

Unspecified
Gramicidin

- Gramicidin D is 1393-88-0
- But neither CAS Number has a structure!

Gramicidin

From Wikipedia, the free encyclopedia

Gramicidin is a heterogeneous mixture of three antibiotic compounds, **gramicidins A, B and C**, making up 80%, 6% and 14%, respectively,^[1] all of which are obtained from the soil bacterial species *Bacillus brevis* and called collectively **gramicidin D**. Gramicidin D contains linear pentadecapeptides, that is chains made up of 15 amino acids.^[2] This is in contrast to **gramicidin S**, which is a cyclic peptide chain.

1. 1393-88-0



~502



~6



Substance
Image
Cannot Be
Displayed
1393-88-0

Unspecified
Gramicidin D

- I have a 1000 CAS Numbers (or Names) – are 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?

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		

Supporting NTA Applications



Exposure surveillance

- What chemicals are in food, products, dust, blood, etc.?



• Chemical prioritization

- What are relevant chemicals & mixtures?



• Exposure forensics

- What are chemical signatures of exposure sources?



• Effect-directed analysis

- What are the biologically active chemicals in complex mixtures?



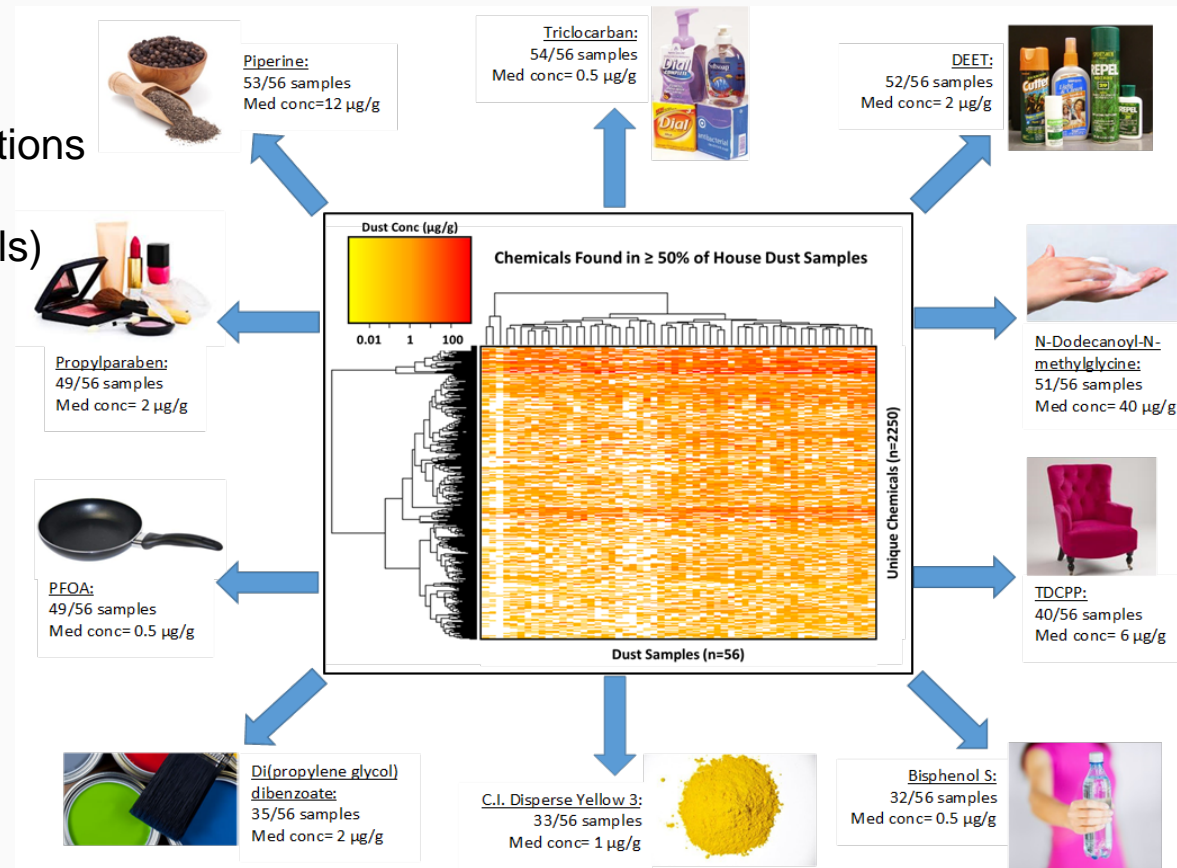
• Biomarker discovery

- What chemicals are predictive of bioactivity/health impairment?



Suspect Screening Analysis Chemicals in House Dust

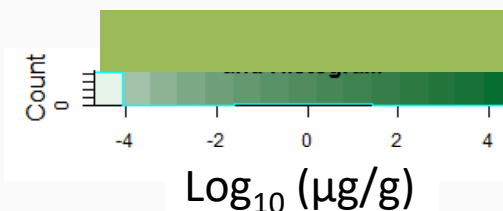
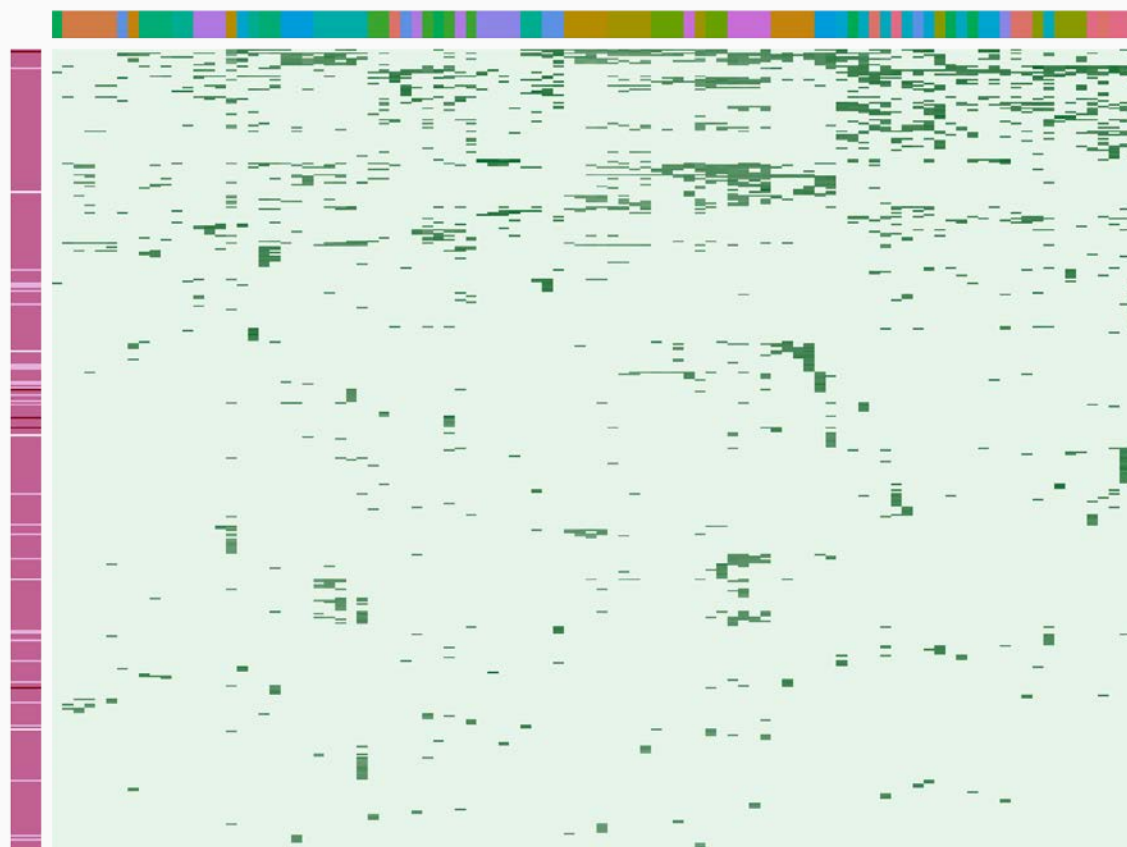
- Chemical confirmation from ToxCast
- Detection frequency
- External calibration for concentrations
- Cluster analysis (homes/chemicals)
- Chemical functional use



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

Batch Searching MS-Ready Formulae

Batch Search

Please enter one identifier per line

Select Input Type(s)

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



This search is based on what we refer to as "Mass Spec Ready Formulae". All chemicals within the database are treated in a manner that all are desalted and stereochemistry is removed as Mass Spectrometry detects the major components of a salt and is insensitive to stereochemistry. As an example, a search for the formula associated with phenol will return phenol, sodium phenolate and calcium phenoxide.

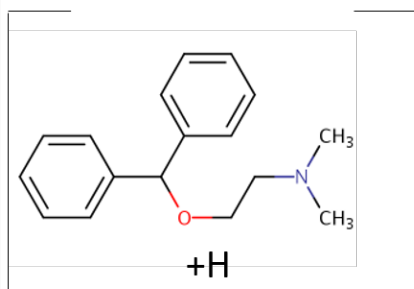
Enter Identifiers to Search

Display All Chemicals

Download Chemical Data

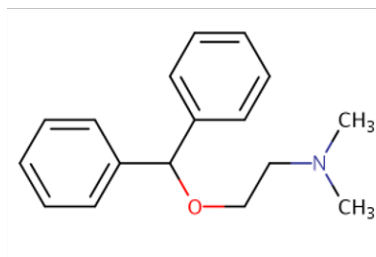
MS-Ready database searching

A) Molecular Ion



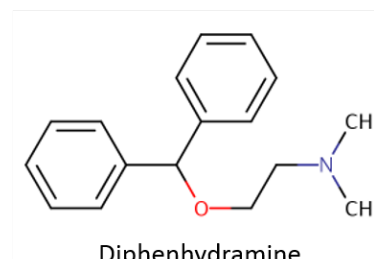
$m/z \approx 256.170$

B) MS-Ready Form

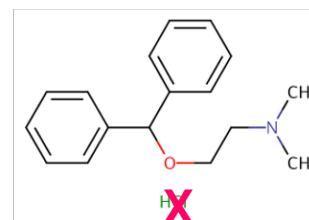


monoisotopic mass= 255.162
C17H21NO
DTXCID802949

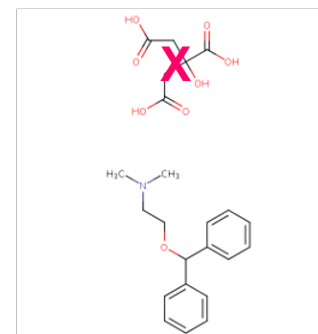
C) Mappings from MS-Ready



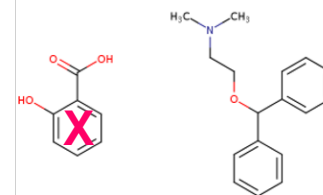
Diphenhydramine
C17H21NO
DTXSID4022949



Diphenhydramine
hydrochloride
C17H22ClNO
DTXSID4020537



Diphenhydramine citrate
C23H29NO8
DTXSID80237211



Diphenhydramine salicylate
C24H27NO4
DTXSID10225883

Atrazine Phenol PFOA

C₈H₁₄CIN₅ C₆H₆O C₈HF₁₅O₂

ChemistryDashboard-AdvancedSearch_2017-11-25_16_50_46.xls [Compatibility Mode] - Excel

INPUT	DTXSID	PREFERRED NAME	MOL FORMULA
C ₈ H ₁₄ CIN ₅	DTXSID9020112	Atrazine	C ₈ H ₁₄ CIN ₅
C ₈ H ₁₄ CIN ₅	DTXSID90237343	Toxurazine	C ₁₈ H ₂₅ Cl ₄ N ₉ O ₂
C ₈ H ₁₄ CIN ₅	DTXSID00187906	GS 18183	C ₈ H ₁₄ CIN ₅
C ₈ H ₁₄ CIN ₅	DTXSID10209527	Atrazine mixture with pendimethalin	C ₂₁ H ₃₃ CIN ₈ O ₄
C ₈ H ₁₄ CIN ₅	DTXSID70230473	Atrazine mixture with terbutryn	C ₁₈ H ₃₃ CIN ₁₀ S
C ₈ H ₁₄ CIN ₅	DTXSID20215154	Maizor	C ₂₁ H ₂₈ ClF ₃ N ₈ O ₄
C ₈ H ₁₄ CIN ₅	DTXSID60192556	1,3,5-Triazine-2,4-diamine, 6-chloro-N,N'-diethyl-, mixt. with 6-chloro-N-ethyl-N'-(1-methylethyl)-1,3,5-triazine-2,4-diamine	C ₁₅ H ₂₆ Cl ₂ N ₁₀
C ₈ H ₁₄ CIN ₅	DTXSID70192527	Acetic acid, (2,4,5-trichlorophenoxy)-, mixt. with 6-chloro-N-ethyl-N'-(1-methylethyl)-1,3,5-triazine-2,4-diamine	C ₁₆ H ₁₉ Cl ₄ N ₅ O ₃
C ₈ H ₁₄ CIN ₅	DTXSID90230576	Agelon	C ₁₈ H ₃₃ CIN ₁₀ S
C ₈ H ₁₄ CIN ₅	DTXSID00222508	Polytriazine	C ₂₄ H ₄₂ Cl ₃ N ₁₅
C ₆ H ₆ O	DTXSID5021124	Phenol	C ₆ H ₆ O
C ₆ H ₆ O	DTXSID4027072	Sodium phenolate	C ₆ H ₅ NaO
C ₆ H ₆ O	DTXSID8073261	Furan, 2-ethenyl-	C ₆ H ₆ O
C ₆ H ₆ O	DTXSID7029322	Phenol, compd. with 2,2',2''-nitrotris[ethanol] (1:1)	C ₁₂ H ₂₁ NO ₄
C ₆ H ₆ O	DTXSID10183353	Oxepin	C ₆ H ₆ O
C ₆ H ₆ O	DTXSID10219242	2-Propynyl ether	C ₆ H ₆ O
C ₆ H ₆ O	DTXSID4074061	Phenol, compd. with 2,3,4,6,7,8,9,10-octahydropyrimido[1,2-a]azepine (1:1)	C ₁₅ H ₂₂ N ₂ O
C ₆ H ₆ O	DTXSID60230144	Tcp (antiseptic)	C ₁₃ H ₁₂ Cl ₂ I ₂ O ₄
C ₆ H ₆ O	DTXSID7064073	Phenol, ammonium salt	C ₆ H ₉ NO
C ₆ H ₆ O	DTXSID10206632	Calcium phenoxide	C ₁₂ H ₁₀ CaO ₂
C ₈ HF ₁₅ O ₂	DTXSID8031865	PFOA	C ₈ HF ₁₅ O ₂
C ₈ HF ₁₅ O ₂	DTXSID8037708	PFOA, ammonium salt	C ₈ H ₄ F ₁₅ NO ₂
C ₈ HF ₁₅ O ₂	DTXSID40880025	Sodium perfluorooctanoate	C ₈ F ₁₅ NaO ₂
C ₈ HF ₁₅ O ₂	DTXSID00880026	Potassium perfluorooctanoate	C ₈ F ₁₅ KO ₂
C ₈ HF ₁₅ O ₂	DTXSID00880127	Silver perfluorooctanoate	C ₈ AgF ₁₅ O ₂
C ₈ HF ₁₅ O ₂	DTXSID50562865	2,2,3,3,4,4,5,5,6,6,7,7,7-Dodecafluoro-6-(trifluoromethyl)heptanoic acid	C ₈ HF ₁₅ O ₂
C ₈ HF ₁₅ O ₂	DTXSID50712909	Pentadecafluorooctanoic acid--piperazine (1/1)	C ₁₂ H ₁₁ F ₁₅ N ₂ O ₂
C ₈ HF ₁₅ O ₂	DTXSID60293633	pentadecafluorooctanoic acid- 1-phenylpiperazine(1:1)	C ₁₈ H ₁₅ F ₁₅ N ₂ O ₂
C ₈ HF ₁₅ O ₂	DTXSID70562266	Pentadecafluorooctanoic acid--pyridine (1/1)	C ₁₃ H ₆ F ₁₅ NO ₂

Chemistry Dashboard Output

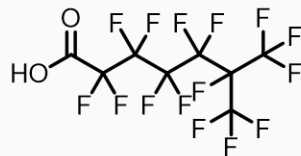


Predicted
molecular
feature,
neutral formula

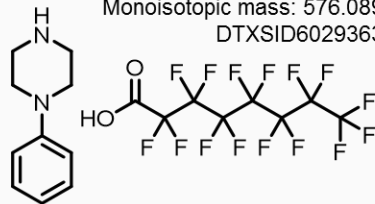
PFOA, C₈H₄F₁₅O₂
Monoisotopic mass: 413.9737
DTXSID8031865



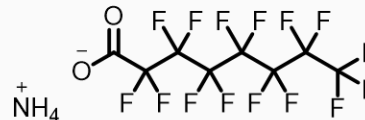
PFOA (isomer), C₈H₄F₁₅O₂
Monoisotopic mass: 413.9737
DTXSID50562865



PFOA-Ph-piperazine, C₁₈H₁₅F₁₅N₂O₂
Monoisotopic mass: 576.0894
DTXSID60293633



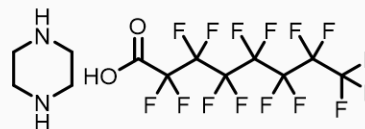
PFOA-NH₄⁺, C₈H₄F₁₅NO₂
Monoisotopic mass: 431.0003
DTXSID8037708



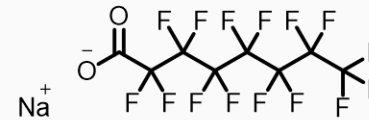
PFOA-Ag⁺, C₈AgF₁₅NO₂
Monoisotopic mass: 519.8710
DTXSID00880127



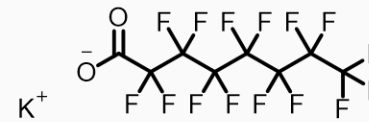
PFOA-piperazine, C₁₂H₁₁F₁₅N₂O₂
Monoisotopic mass: 500.0581
DTXSID50712909



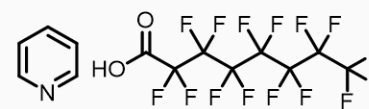
PFOA-Na⁺, C₈F₁₅NaO₂
Monoisotopic mass: 435.9557
DTXSID40880025



PFOA-K⁺, C₈F₁₅KO₂
Monoisotopic mass: 451.9296
DTXSID00880026



PFOA-pyridine, C₁₃H₆F₁₅NO₂
Monoisotopic mass: 493.0159
DTXSID70562266



Chemistry Dashboard Output



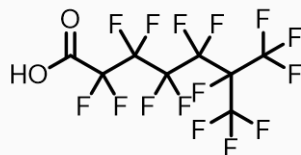
Predicted
molecular
feature,
neutral formula

Two structures
to one formula

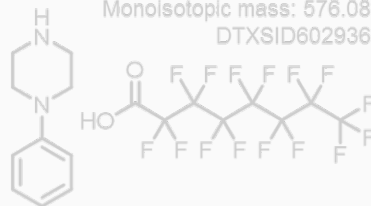
PFOA, $\text{C}_8\text{HF}_{15}\text{O}_2$
Monoisotopic mass: 413.9737
DTXSID8031865



PFOA (isomer), $\text{C}_8\text{HF}_{15}\text{O}_2$
Monoisotopic mass: 413.9737
DTXSID50562865



PFOA-Ph-piperazine, $\text{C}_{18}\text{H}_{15}\text{F}_{15}\text{N}_2\text{O}_2$
Monoisotopic mass: 576.0894
DTXSID60293633



PFOA- NH_4^+ , $\text{C}_8\text{H}_4\text{F}_{15}\text{NO}_2$
Monoisotopic mass: 431.0003
DTXSID8037708



PFOA- Ag^+ , $\text{C}_8\text{AgF}_{15}\text{NO}_2$
Monoisotopic mass: 519.8710
DTXSID00880127



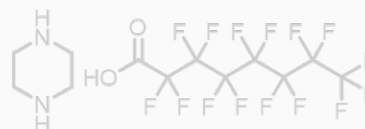
PFOA- Na^+ , $\text{C}_8\text{F}_{15}\text{NaO}_2$
Monoisotopic mass: 435.9557
DTXSID40880025



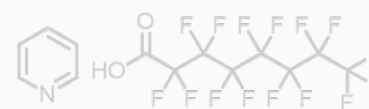
PFOA- K^+ , $\text{C}_8\text{F}_{15}\text{KO}_2$
Monoisotopic mass: 451.9296
DTXSID00880026



PFOA-piperazine, $\text{C}_{12}\text{H}_{11}\text{F}_{15}\text{N}_2\text{O}_2$
Monoisotopic mass: 500.0581
DTXSID50712909



PFOA-pyridine, $\text{C}_{13}\text{H}_5\text{F}_{15}\text{NO}_2$
Monoisotopic mass: 493.0159
DTXSID70562266



Chemistry Dashboard Output



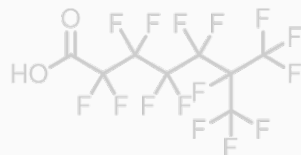
Exclude salts &
counter-ions

Adds H to
neutralize,
maps salt form
of structure to
neutral formula

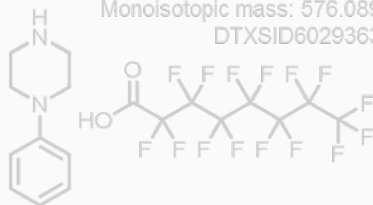
PFOA, $C_8H_4F_{15}O_2$
Monoisotopic mass: 413.9737
DTXSID8031865



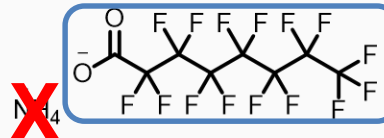
PFOA (isomer), $C_8H_4F_{15}O_2$
Monoisotopic mass: 413.9737
DTXSID50562865



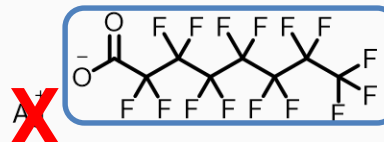
PFOA-Ph-piperazine, $C_{18}H_{15}F_{15}N_2O_2$
Monoisotopic mass: 576.0894
DTXSID60293633



PFOA- NH_4^+ , $C_8H_4F_{15}NO_2$
Monoisotopic mass: 431.0003
DTXSID8037708



PFOA- Ag^+ , $C_8AgF_{15}NO_2$
Monoisotopic mass: 519.8710
DTXSID00880127



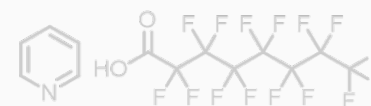
PFOA- Na^+ , $C_8F_{15}NaO_2$
Monoisotopic mass: 435.9557
DTXSID40880025



PFOA- K^+ , $C_8F_{15}KO_2$
Monoisotopic mass: 451.9296
DTXSID00880026



PFOA-pyridine, $C_{13}H_5F_{15}NO_2$
Monoisotopic mass: 493.0159
DTXSID70562266



Chemistry Dashboard Output



Separates
components
within mixture

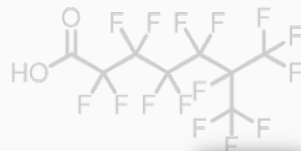
PFOA in
mixture
mapped to
neutral formula,

Heterocycles
are separate,
searchable
components

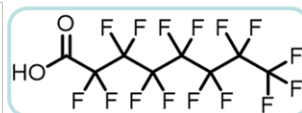
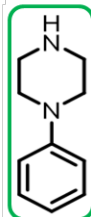
PFOA, C₈HF₁₅O₂
Monoisotopic mass: 413.9737
DTXSID8031865



PFOA (isomer), C₈HF₁₅O₂
Monoisotopic mass: 413.9737
DTXSID50562865



PFOA · Ph-piperazine, C₈HF₁₅O₂ C₁₀H₁₄N₂
Monoisotopic masses: 413.9737 + 162.1157
DTXSID8031865, DTXSID8057855



PFOA-NH₄⁺, C₈H₄F₁₅NO₂
Monoisotopic mass: 431.0003
DTXSID8037708



PFOA-Ag⁺, C₈AgF₁₅NO₂
Monoisotopic mass: 519.8710
DTXSID00880127



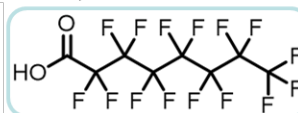
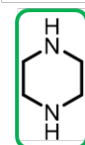
PFOA-Na⁺, C₈F₁₅NaO₂
Monoisotopic mass: 435.9557
DTXSID40880025



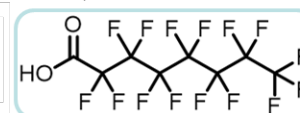
PFOA-K⁺, C₈F₁₅KO₂
Monoisotopic mass: 451.9296
DTXSID00880026



PFOA · Piperazine, C₈HF₁₅O₂ C₄H₁₀N₂
Monoisotopic masses: 413.9737 + 86.0844
DTXSID8031865, DTXSID1021164



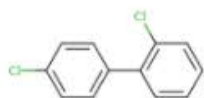
PFOA · Pyridine, C₈HF₁₅O₂ C₅H₅N₂
Monoisotopic masses: 413.9737 + 79.0422
DTXSID8031865, DTXSID9021924



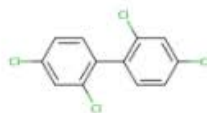
- Sometimes the simplest of questions are difficult to answer!
 - What is the list of CAS Numbers for all PCBs?
 - Can I get an SDF file of all PCBs?
 - Do you have predicted properties for all PCBs?
 - What toxicity data is available for individual PCBs?
 - Have you measured ToxCast data for any PCBs?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

Chemical “Families”

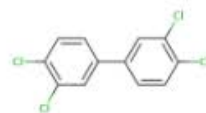
Download as: [TSV](#) [Excel](#) [SDF](#)



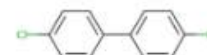
2,4'-Dichlorobiphenyl
34863-43-7



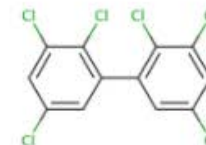
2,2',4,4'-Tetrachlorobiphenyl
2437-79-8



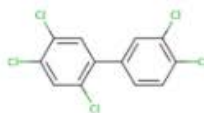
3,3',4,4'-Tetrachlorobiphenyl
32598-13-3



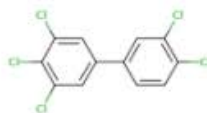
4,4'-Dichlorobiphenyl
2050-68-2



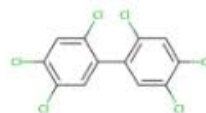
2,2',3,3',5,5'-Hexachlorobiphenyl
35694-04-3



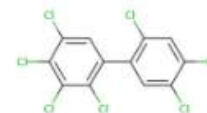
2,3',4,4',5-Pentachlorobiphenyl
31508-00-6



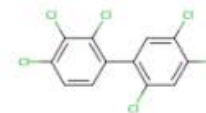
3,3',4,4',5-Pentachlorobiphenyl
57465-28-8



2,2',4,4',5,5'-Hexachlorobiphenyl
35065-27-1



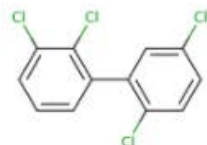
2,2',3,4,4',5,5'-Heptachlorobiphenyl
35065-29-3



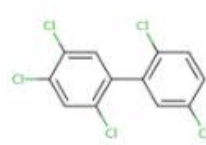
2,2',3,4,4',5'-Hexachlorobiphenyl
35065-26-2



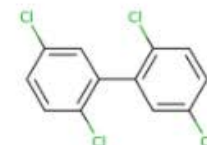
2,2',3,5,6-Pentachlorobiphenyl
36379-99-6



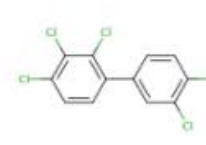
2,2',3,5'-tetrachlorobiphenyl
41464-39-5



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
1	DTXSID	CASRN	PREFERRED NAME	IUPAC NAME	MOLECULAR F	MONOISOT	AVERAGE	SMILES	INCHI KEY
2	DTXSID9074779	70362-45-7	PCB 045	2,2',3,6-Tetrachloro-1,1'-biphenyl	C12H6Cl4	289.92236	291.98001	<chem>C1C1=CC=C(C1)C(=C1C1)C1=CC=CC=C1C1</chem>	VHGHZT
3	DTXSID9074777	38444-73-4	PCB 019	2,2',6-Trichloro-1,1'-biphenyl	C12H7Cl3	255.96133	257.54001	<chem>C1C1=CC=CC(C1)=C1C1=C(C1)C=CC=C1</chem>	MXVJRBBC
4	DTXSID9074228	74472-39-2	2,3',4',5',6-Pentachlorobiphenyl	2,3',4',5',6-Pentachlorobiphenyl	C12H5Cl5	323.88339	326.42001	<chem>C1C1=CC(=CC(C1)=C1C1)C1=C(C1)C=CC=C1C1</chem>	WAZUWHG
5	DTXSID9074226	74472-37-0	2,3,4,4',5-Pentachlorobiphenyl	2,3,4,4',5-Pentachlorobiphenyl	C12H5Cl5	323.88339	326.42001	<chem>C1C1=CC=C(C=C1)C1=C(C1)C(C1)=C(C1)C(C1)=C1</chem>	SXZSFWHC
6	DTXSID9074224	74472-35-8	2,3,3',4,6-Pentachlorobiphenyl	2,3,3',4,6-Pentachlorobiphenyl	C12H5Cl5	323.88339	326.42001	<chem>C1C1=CC=CC(=C1)C1=C(C1)C(C1)=C(C1)C=C1C1</chem>	XGQBSVVY
7	DTXSID9074222	74472-33-6	2,3,3',6-Tetrachlorobiphenyl	2,3,3',6-Tetrachlorobiphenyl	C12H6Cl4	289.92236	291.98001	<chem>C1C1=CC=CC(=C1)C1=C(C1)C(C1)=CC=C1C1</chem>	WZNAMGY
8	DTXSID9074220	74338-23-1	2,3',5',6-Tetrachlorobiphenyl	2,3',5',6-Tetrachlorobiphenyl	C12H6Cl4	289.92236	291.98001	<chem>C1C1=CC(=CC(C1)=C1)C1=C(C1)C=CC=C1C1</chem>	HDULUCZR
9	DTXSID9074199	68194-11-6	2,3,4',5,6-Pentachlorobiphenyl	2,3,4',5,6-Pentachlorobiphenyl	C12H5Cl5	323.88339	326.42001	<chem>C1C1=CC=C(C=C1)C1=C(C1)C(C1)=CC(C1)=C1C1</chem>	ZDDZPDTV
10	DTXSID9074197	68194-08-1	2,2',3,4',6-Hexachlorobiphenyl	2,2',3,4',6-Hexachlorobiphenyl	C12H4Cl6	357.84442	360.85999	<chem>C1C1=CC(C1)=C(C(C1)=C1)C1=C(C1)C(C1)=CC=C1C1</chem>	RPPNJBZN
11	DTXSID9074195	68194-04-7	2,2',4,6-Tetrachlorobiphenyl	2,2',4,6-Tetrachlorobiphenyl	C12H6Cl4	289.92236	291.98001	<chem>C1C1=CC=C(C(C1)=C1)C1=C(C1)C=CC=C1C1</chem>	WVHNUGR
12	DTXSID9074193	60233-25-2	2,2',3,4',6-Pentachlorobiphenyl	2,2',3,4',6-Pentachlorobiphenyl	C12H5Cl5	323.88339	326.42001	<chem>C1C1=CC(C1)=C(C(C1)=C1)C1=C(C1)C(C1)=CC=C1</chem>	GOFFZTAP
13	DTXSID9074191	60145-23-5	2,2',3,4,4',5,6-Heptachlorobiphenyl	2,2',3,4,4',5,6-Heptachlorobiphenyl	C12H3Cl7	391.80544	395.31	<chem>C1C1=CC(C1)=C(C(C1)=C1)C1=C(C1)C(C1)=C(C1)C(C1)=C1</chem>	RXRLRYZU
14	DTXSID9074149	41411-61-4	2,2',3,4,5,6-Hexachlorobiphenyl	2,2',3,4,5,6-Hexachlorobiphenyl	C12H4Cl6	357.84442	360.85999	<chem>C1C1=C(C=C1)C1=C(C1)C(C1)=C(C1)C(C1)=C1C1</chem>	RUEIBQJF
15	DTXSID9074147	40186-70-7	2,2',3,3',4,5',6-Heptachlorobiphenyl	2,2',3,3',4,5',6-Heptachlorobiphenyl	C12H3Cl7	391.80544	395.31	<chem>C1C1=CC(C1)=C(C1)C(=C1)C1=C(C1)C(C1)=C(C1)C=C1C1</chem>	KJBDZJFS
16	DTXSID9074145	39635-33-1	3,3',4,5,5'-Pentachlorobiphenyl	3,3',4,5,5'-Pentachlorobiphenyl	C12H5Cl5	323.88339	326.42001	<chem>C1C1=CC(=CC(C1)=C1)C1=CC(C1)=C(C1)C(C1)=C1</chem>	MXVAYAXI
17	DTXSID9074143	38444-76-7	2,3',6-Trichlorobiphenyl	2,3',6-Trichlorobiphenyl	C12H7Cl3	255.96133	257.54001	<chem>C1C1=CC=CC(=C1)C1=C(C1)C=CC=C1C1</chem>	VQOFJPFY
18	DTXSID9074141	38380-05-1	2,2',3,3',4,6'-Hexachlorobiphenyl	2,2',3,3',4,6'-Hexachlorobiphenyl	C12H4Cl6	357.84442	360.85999	<chem>C1C1=CC=C(C1)C(=C1C1)C1=C(C1)C(C1)=C(C1)C=C1</chem>	OKBJVIVE
19	DTXSID9073599	65510-45-4	2,2',3,4,4'-Pentachlorobiphenyl	2,2',3,4,4'-Pentachlorobiphenyl	C12H5Cl5	323.88339	326.42001	<chem>C1C1=CC(C1)=C(C=C1)C1=C(C1)C(C1)=C(C1)C=C1</chem>	LACXVZHA
20	DTXSID9073541	52744-13-5	2,2',3,3',5,6'-Hexachlorobiphenyl	2,2',3,3',5,6'-Hexachlorobiphenyl	C12H4Cl6	357.84442	360.85999	<chem>C1C1=CC(=C(C1)C(C1)=C1)C1=C(C1)C(C1)=CC=C1C1</chem>	UUTNFLRS
21	DTXSID9073410	16606-02-3	2,4',5-Trichlorobiphenyl	2,4',5-Trichlorobiphenyl	C12H7Cl3	255.96133	257.54001	<chem>C1C1=CC=C(C=C1)C1=C(C1)C=CC(C1)=C1</chem>	VAHKBZSA
22	DTXSID80873557	36559-22-5	2,2',3,4'-Tetrachlorobiphenyl	2,2',3,4'-Tetrachlorobiphenyl	C12H6Cl4	289.92236	291.98	<chem>C1C1=CC(C1)=C(C=C1)C1=CC=CC(C1)=C1C1</chem>	ALFHIHDQ
23	DTXSID8074780	61798-70-7	PCB 131	2,2',3,3',4,6-Hexachlorobiphenyl	C12H4Cl6	357.84442	360.85999	<chem>C1C1=CC(C1)=C(C1)C(C1)=C1C1=CC=CC(C1)=C1C1</chem>	WDLTVNW
24	DTXSID8074239	74472-51-8	2,3,3',4,4',5,6'-Heptachlorobiphenyl	2,3,3',4,4',5,6'-Heptachlorobiphenyl	C12H3Cl7	391.80544	395.31	<chem>C1C1=CC(=CC(C1)=C1)C1=C(C1)C(C1)=C(C1)C(C1)=C1C1</chem>	ZUTDUGMH
25	DTXSID8074237	74472-49-4	2,2',3,4,5,6,6'-Heptachlorobiphenyl	2,2',3,4,5,6,6'-Heptachlorobiphenyl	C12H3Cl7	391.80544	395.31	<chem>C1C1=CC=CC(C1)=C1C1=C(C1)C(C1)=C(C1)C(C1)=C1C1</chem>	FGDPOTMH
26	DTXSID8074235	74472-47-2	2,2',3,4,4',5,6-Heptachlorobiphenyl	2,2',3,4,4',5,6-Heptachlorobiphenyl	C12H3Cl7	391.80544	395.31	<chem>C1C1=CC(C1)=C(C=C1)C1=C(C1)C(C1)=C(C1)C(C1)=C1C1</chem>	DJEUXBQA
27	DTXSID8074233	74472-44-9	2,3,3',4',5,6-Hexachlorobiphenyl	2,3,3',4',5,6-Hexachlorobiphenyl	C12H4Cl6	357.84442	360.85999	<chem>C1C1=CC=C(C=C1C1)C1=C(C1)C(C1)=CC(C1)=C1C1</chem>	ZAGRQXMH

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: 1336-36-3

Name: Polychlorinated biphenyls

Substance Type: Mixture/Formulation

QC Level: DSSTox_High

Data Source: STN(DSSTox)

QC Notes: biphenyl with multiple (unknown number) chlorines attached at unknown locations

Compound_ID:

Chemical Shown:

No Structure

Private Notes:

Source of CAS-Compound:

Double Stereo:

Chiral Stereo:

Chemical Form:

► Synonyms (31)

► Other Cas (0)

▼ Successor Substances (209)

	CAS-RN	Relationship	Source	Struc	Casrn	Comments
●	32774-16-6	is a Representative Isomer of this	STN(DSSTox)	✓	■	structure shown 3,3',4,4',5,5'
●	2051-60-7	is a Representative Isomer of this	Public	■	■	
●	2051-61-8	is a Representative Isomer of this	Public	■	■	
●	2051-62-9	is a Representative Isomer of this	Public	■	■	
●	13029-08-8	is a Representative Isomer of this	Public	■	■	
●	16605-91-7	is a Representative Isomer of this	Public	■	■	
●	25569-80-6	is a Representative Isomer of this	Public	■	■	
●	33284-50-3	is a Representative Isomer of this	Public	■	■	

Relationship Mappings

- 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 assays)



The screenshot shows the EPA website's navigation bar with links for Environmental Topics, Laws & Regulations, and About EPA. Below this is the TSCA Chemical Substance Inventory page. The page title is "TSCA Chemical Substance Inventory". On the left is a sidebar with links: TSCA Inventory Home, About the Inventory, Access the Inventory, and Policy and Guidance. The main content area has the title "Chemical Substances of Unknown or Variable Composition, Complex Reaction Products and Biological Materials (UVCB Substance) on the TSCA Inventory". Below the title is a paragraph: "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."

Environmental Topics Laws & Regulations About EPA Search EPA.gov

TSCA Chemical Substance Inventory

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[TSCA Inventory Home](#)
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[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

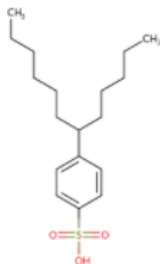
i Searched by Synonym: Found 1 result for
'Linear alkylbenzene sulfonate'.

Presence in Lists

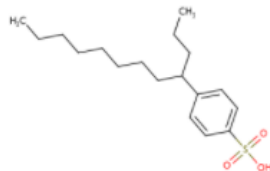
Surfactant List Screened in Swiss Wastewater (2014)

Surfactant List Screened in Swiss Wastewater (2014)

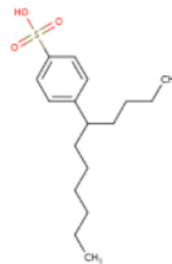
EAWAGSURF is a list of surfactants screened in Swiss wastewater effluents as part of a 2014 study. Structures/mixtures are being progressively curated and linked (Schymanski/Williams). Further details in Schymanski et al 2014, DOI: 10.1021/es4044374



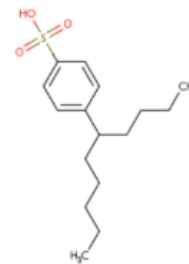
4-(Dodecan-6-yl)benzene-1-sulfon...
23003-92-1



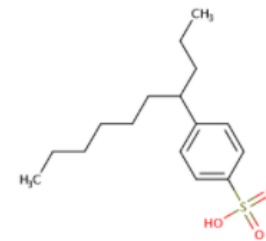
4-(dodecan-4-yl)benzene-1-sulfoni...
NOCAS_862870



C11-LAS
NOCAS_881097



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



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

Ambiguous Chemicals

Chemistry Dashboard

Submit Comment

Copy

Aa

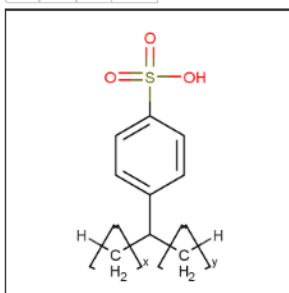
Aa

Aa

Alkylbenzenesulfonate, linear

42615-29-2 | DTXSID3020041

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



Intrinsic Properties

Molecular Formula: $(CH_2)_x(CH_2)_yC_7H_8O_3S$

Find All Chemicals

Average Mass: Not Found

Monoisotopic Mass: Not Found

Structural Identifiers

Linked Substances

Presence in Lists

Record Information

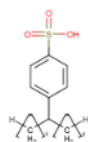
Related Substances

Chemical Properties

Analytical

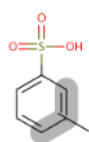
Comments

Searched Chemical



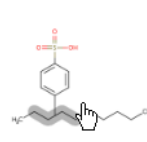
Alkylbenzenesulfonate, linear
42615-29-2

SUCCESSOR:Representative Component



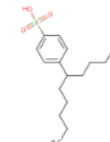
(C10-C18) Alkylbenzenesulfonic acid
68584-22-5

SUCCESSOR:Representative Component



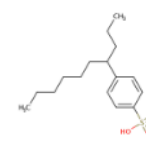
C10-linear alkylbenzenesulfonate
NOCAS_891689

SUCCESSOR:Representative Component



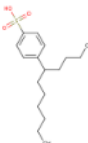
4-(decan-5-yl)benzene-1-sulfonic acid
NOCAS_881148

SUCCESSOR:Representative Component



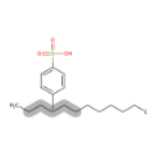
4-(decan-4-yl)benzenesulfonic acid
NOCAS_891333

SUCCESSOR:Representative Component



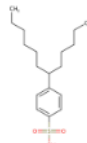
4-(undecan-5-yl)benzene-1-sulfonic acid
NOCAS_881097

SUCCESSOR:Representative Component



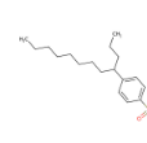
C12-linear alkyl benzene sulfonate
NOCAS_891641

SUCCESSOR:Representative Component



4-(Dodecan-8-yl)benzene-1-sulfonic acid
23003-92-1

SUCCESSOR:Representative Component



4-(dodecan-4-yl)benzene-1-sulfonic acid
NOCAS_882870

SUCCESSOR:General Form

No Chemical
Structure
Associated
with this
Substance

Benzenesulfonic acid, C10-13-alkyl derivs., sodium ...
68411-30-3

SUCCESSOR:General Form

No Chemical
Structure
Associated
with this

SUCCESSOR:General Form

No Chemical
Structure
Associated
with this

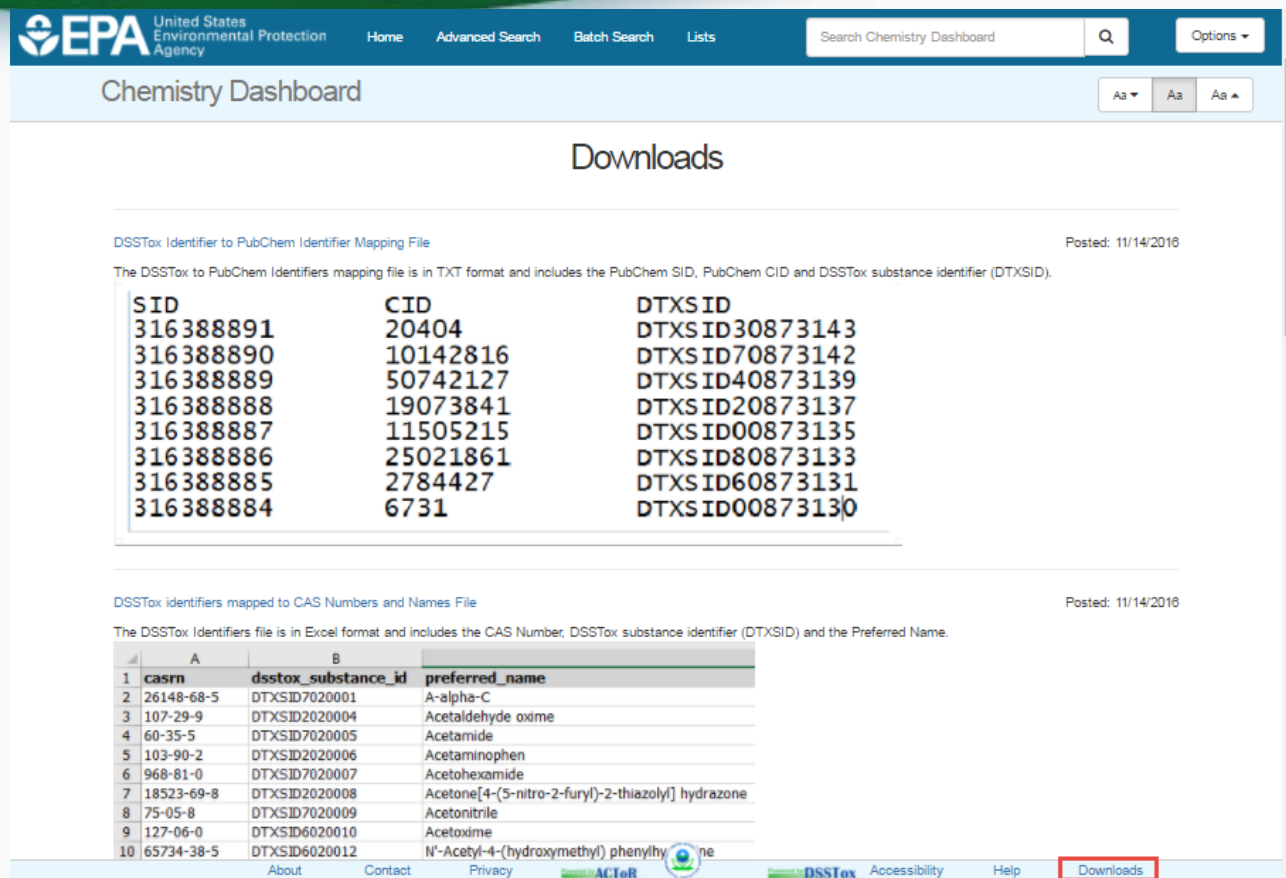
SUCCESSOR:General Form

No Chemical
Structure
Associated
with this

SUCCESSOR:Representative Component

No Chemical
Structure
Associated
with this

Delivering our Chemistry Data



The screenshot shows the EPA Chemistry Dashboard with a 'Downloads' section. It features two download links: 'DSSTox Identifier to PubChem Identifier Mapping File' and 'DSSTox identifiers mapped to CAS Numbers and Names File'. The first link includes a table of identifiers. The second link includes a table of identifiers mapped to CAS numbers and names. The 'Downloads' link in the footer is highlighted with a red box.

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	
	casrn	dsstox_substance_id	preferred_name
1	casrn	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

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

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](#)

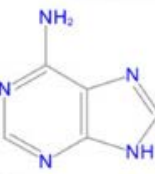
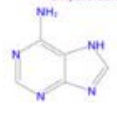
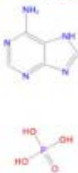
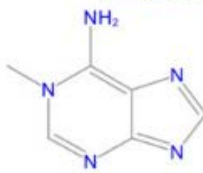
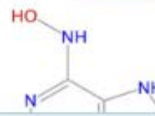
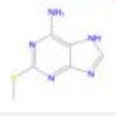
Screenshots

iPhone | iPad

Carrier 2:30 PM

+ m/z Name ¹³C 17

adenine

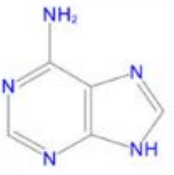

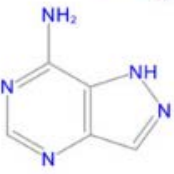
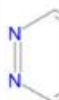

73-24-5 Adenine 1H-Purin-6-amine	73663-94-2 Adenine, dihydride Adenine dihydride
	
135.05450	390.87908
52175-10-7 Adenine phosphate EINECS 257-702-7	5142-22-3 1-Methyladenine Adenine, 1-methyl-
	
233.03139	149.07015
19152-67-1 Adenine, 2-chloro-N- 2-Chloro-N-hydroxyadenine	62700-65-6 Purine, 6-amino-2- methythio-, hydrochloride Adenine, 2-methylthio- hydrochloride
	

Carrier 2:31 PM

+ m/z Name ¹³C

m/z 135.0545

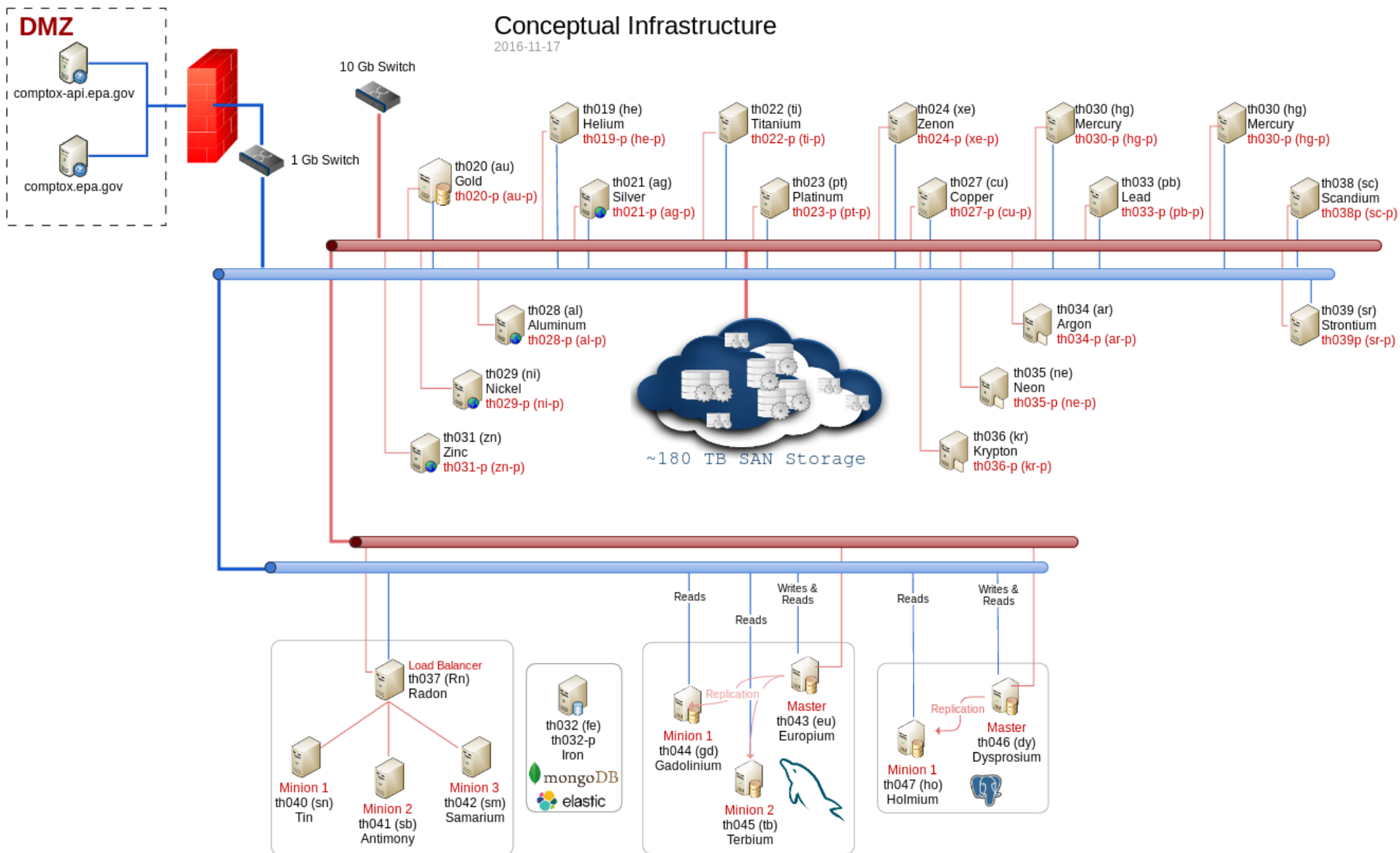
¹³C Example: 25 32.4 115 (ppm)

73-24-5 Adenine 1H-Purin-6-amine	2380-6
	
135.05450 Δ 0.00000	135.05
13877-56-0 7-Aminopurazole(4,3- 7-Aminopurazole(4,3-di- pyrimidine	160568
	
135.05450 Δ 0.00000	135.05
452-06-2 2-Aminopurine EINECS 207-197-4	5019-45
	

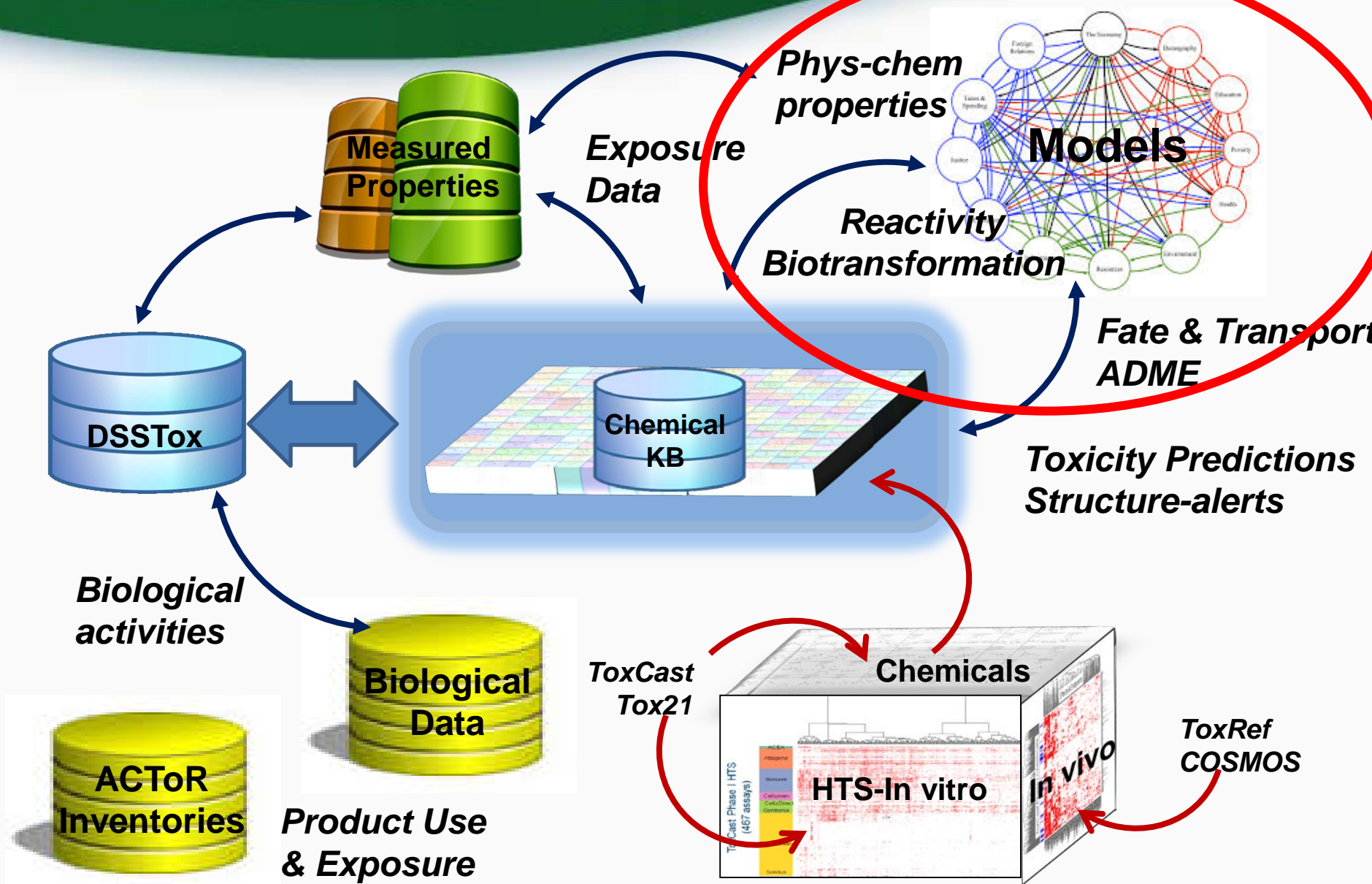
Computational Infrastructure and Processes

- 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



We're not done yet...



NTA Support Using Fragmentation Predictions



- Work in progress
 - Chemical structures for all chemicals processed into “MS-ready” form
 - MS fragmentation - +ve/-ve ESI spectra low (10V), medium (20V) and high (40V) collision energy levels plus EI data
 - All data generated and presently building spectral search interface

T.E.S.T services (ALPHA)

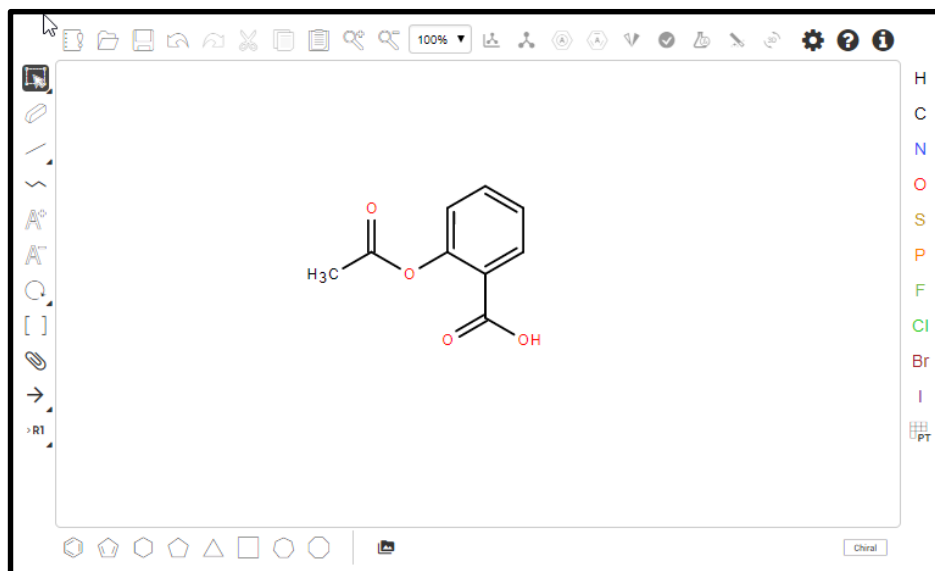
- 96hr fathead minnow 50% lethal concentration (LC50)
- 48hr daphnia magna 50% lethal concentration (LC50)
- Tetrahymena pyriformis 50% growth inhibition conc. (IGC50)
- Oral rat 50% lethal dose (LD50)
- Bioconcentration Factor (BCF)
- Developmental Toxicity (DevTox)
- Ames Mutagenicity (Mutagenicity)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

Real time predictions

Chemistry Dashboard

Aa ▾ Aa Aa ▴

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

“RapidTox” prioritization

<https://tinyurl.com/y7bkxxt3>



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 Notice

New Chemicals Review Program Implementation and Approaches for Identifying Potential Candidates for Prioritization for Existing Chemical Risk Evaluations Under the Amended Toxic Substances Control Act (TSCA); Notice of Public Meetings and Opportunity for Public Comment

A Notice by the [Environmental Protection Agency](#) on 11/06/2017



- “Identifying Potential Candidates for **Prioritization** for Existing Chemical Risk Evaluations Under the Amended Toxic Substances Control Act”
 - Use the data streams under the dashboard – experimental, in vitro, in vivo, predicted physchem, environmental fate, read-across
 - RapidTox: algorithmic-based prioritization of chemical datasets

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

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NRMRL*

NORMAN Network

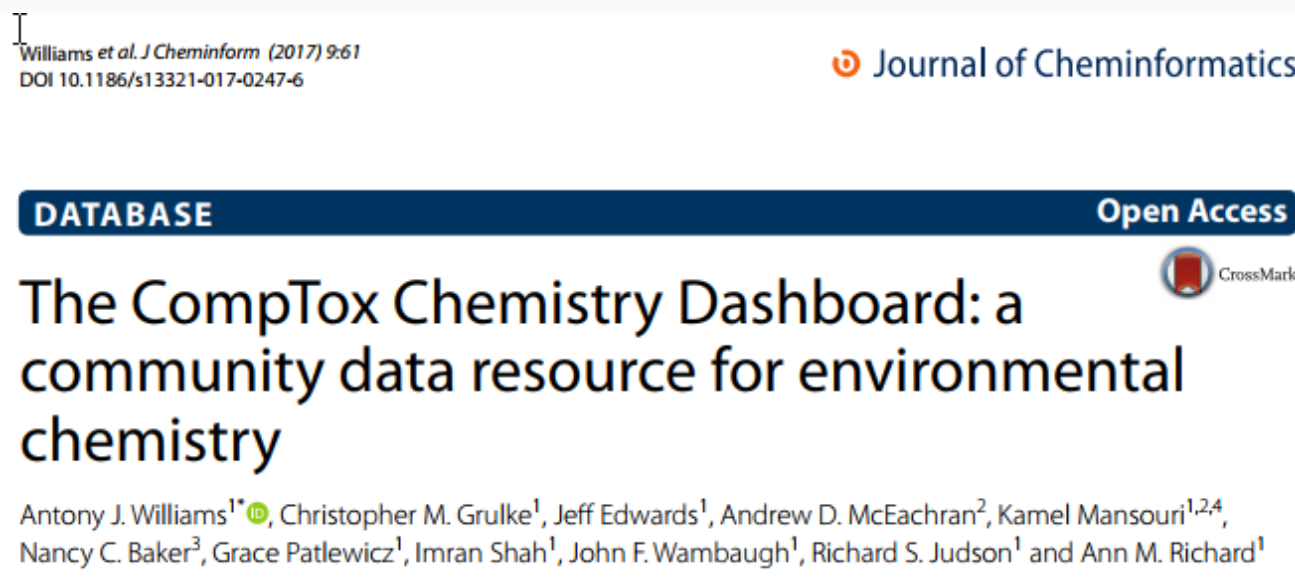
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