

# Delivering chemical-associated data via EPA web applications

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Cheminformatics Resources of U.S. Governmental Organizations– May 11th 2022

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

## The State of Internet Chemistry...



- The past two decades has seen an explosion in online data
- There are so many resources to choose from...so much data
- In our world there are dominant aggregating resources done well: PubChem, ChEMBL, eChemPortal, ECHA
- Do we need yet another online chemistry database?

## 20 Years of Curating Data in Our Team





Mutation Research/Fundamental and Molecular Mechanisms of Mutagenesis Volume 499, Issue 1, 29 January 2002, Pages 27-52



Mutation Research Frontiers

Distributed structure-searchable toxicity (DSSTox) public database network: a proposal

Ann M. Richard ª 🐣 ⊠, ClarLynda R. Williams ª, b

EPA's DSSTox Database: The strategic role and requirements of chemical curation

Ann M. Richard

Center for Computational Toxicology & Exposure Office of Research & Development US Environmental Protection Agency



## The Charge for the CompTox Chemicals Dashboard



- Develop a "first-stop-shop" for environmental chemical data to support EPA and partner decision making:
  - Centralized location for chemical data (DSSTox foundation)
  - Chemistry, exposure, hazard and dosimetry
  - Combination of existing data and predictive models
  - Publicly accessible, periodically updated, curated
- Easy access to data improves efficiency and ultimately accelerates chemical risk assessment

## CompTox Chemicals Dashboard https://comptox.epa.gov/dashboard





#### **Detailed Chemical Pages**





 Chemical page: Wikipedia snippet when available, intrinsic properties, structural identifiers, linked substances

## "Executive Summary" regarding chemical toxicity

**Executive Summary** 

- Quantitative Risk Assessment Values
  - 🕑 IRIS values available 🗹
  - 🖄 No PPRTV values
  - 🔮 EPA RSL values available 🗹

🕑 Minimum RfD:0.0003 mg/kg-day ( chronic, ) 🗹

🕑 Minimum RfC:2e-06 mg/m3 ( chronic, ) 🗹

- Chronic toxicity PODs available
- Subchronic Toxicology
   No subchronic toxicity data available
- Developmental Toxicology
   No developmental toxicity data available
- Acute Toxicology
- 😣 No acute toxicity data available



- Overview of toxicityrelated info
  - Quantitative values
  - Physchem. and Fate & Transport
  - Adverse Outcome Pathway links
  - In vitro bioactivity summary plot



#### **Experimental and Predicted Data**

Summary	~	Q Search Chemical P
🛓 EXPORT 👻		
Property	≡ Experimental average	$\equiv$ Predicted average $\equiv$
Polarizability	-	35.8 (1)
Henry's Law	4.57e-7 (1)	4.59e-7 (1)
Boiling Point	495 (3)	480 (4)
Flash Point	-	234 (2)
Melting Point	177 (8)	189 (3)
Molar Refractivity	-	90.3 (1)
Molar Volume	-	196 (1)
Surface Tension	-	53.9 (2)
Density	-	1.28 (2)
Vapor Pressure	5.49e-9 (1)	3.61e-9 (3)

- Physchem and Fate & Transport experimental and predicted data
- Data extracted (somewhat curated) from literature and databases
- Multiple prediction algorithms used: OPERA, TEST, ACD/Labs, EPI Suite
- Data can be downloaded as Excel, TSV and CSV files



## **Chemical Hazard Data**



## **ToxVal Database**

- >50k chemicals
- >770k tox. values
- >30 sources of data
- ~5k journals cited
- ~70k citations

FU		anture	<u> </u>	Searc	IIIazaiu						Ľ		
ا 🕹	Export 🝷												
ore	Priority 个	Source	≡ Type ≡	Subtype $\equiv$	Risk Assessment	≡ Quali	<sup>ii</sup> Value ∃	Units	Study Type	$_{ m eRoute}^{ m Exposur}\equiv$	Critical effect	∃ Species ☰	Year 📃
Ľ	1	IRIS	LOAEL	-	chronic	=	9.10e-3	mg/m3	-	inhalation	reduced ovulation rate and ovary weight	-	-
L	1	IRIS	LOAEL	-	chronic	=	4.60e-3	mg/m3	-	inhalation	reduced embryo/fetal survival	-	-
∎	3	ECOTOX	NOEL	-	chronic growth	-	100	mg/kg f	Growth	Food	Weight	norway	2000
L ≡	З	ECOTOX	NOEL	-	chronic growth	-	25.0	ul/org	Growth	Topical,	Weight	house	1990
∎	3	ECOTOX	NOEL	-	chronic growth	-	50.0	mg/kg f	Growth	Food	Weight	norway	2000
∎	3	ECOTOX	NOEL	-	chronic growth	-	25.0	ul/org	Growth	Topical,	Weight	house	1990
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Ē	3	ECOTOX	LOEL	-	chronic growth	-	100	mg/kg f	Growth	Food	Weight	norway	2000
Ē	3	ECOTOX	LOEL	-	chronic growth	-	100	mg/kg f	Growth	Food	Weight	norway	2000
Ē	3	ECOTOX	NOEL	-	chronic growth	-	25.0	ul/org	Growth	Topical,	Weight	house	1990
Row	/s: <b>58</b>						Total Rows	s: 58					

## Safety Data – Thank you PubChem! Bring together resources





#### Sources of Exposure to Chemicals



#### Chemical Weight Fractions (CWF)

Q Search Chemical Weig	ght F	ractions												🛓 EXPOR	т •	
Product Name	=	Product Use Category	=	Categorization Subtype	=	Minimum Weight Fraction	=	Maximum Weight Fraction	≡	Data Type	=	Source	=	Product Count	=	
	$\nabla$		$\nabla$		$\nabla$		$\nabla$		$\nabla$		$\nabla$		$\nabla$		$\nabla$	
48743 pah mixture		Not yet Categorized				-		-		reported		SIRI		1		
asphalt cement penetration 60-7	70	Not yet Categorized				-		-		reported		SIRI		1		
base-neutral 4 1ml methylene ch	<u>1</u>	Not yet Categorized				-		-		reported		SIRI		1		
base neutral calibration checkco		Not yet Categorized				-		-		reported		SIRI		1		
benzo (a) pyrene_ 98%_ b1008-0	2	Not yet Categorized				-		-		reported		SIRI		1		
benzo (a) pyrene_ md-1956		Not yet Categorized				0.990		1.00		reported		SIRI		1		
blasocut 2000 cf art no 875		Not yet Categorized				0.00		1.00e-3		reported		SIRI		1		
blasocut 2000 universal_ 870		Not yet Categorized				-		-		reported		SIRI		1		
blasocut 2000 universal art_ 870		Not yet Categorized				0.00		1.00e-3		reported		SIRI		1		
blasocut 4000 strong_ 872		Not yet Categorized				-		-		reported		SIRI		1		
blasocut 4000 universal art_ 872		Not yet Categorized				0.00		1.00e-3		reported		SIRI		1		
clp-011a clp base/neutrals check		Not yet Categorized				-		-		reported		SIRI		1	_	-

### A recent focus on PFAS chemicals



9

0



**Chemical Details** 

#### Perfluorooctanesulfonic acid 1763-23-1 | DTXSID3031864 Searched by DTXSID3031864.

#### Details



#### Wikipedia

Perfluorooctanesulfonic acid (PFOS) (conjugate base perfluorooctanesulfonate) is an anthropogenic (human-made) fluorosurfactant, now regarded as a global pollutant. PFOS was the key ingredient in Scotchgard, a fabric protector made by 3M, and related stain repellents. In many contexts, PFOS refers to the parent sulfonic acid and its various salts of perfluorooctanesulfonate. These are all colorless or white, water soluble solids. Although of low acute toxicity, PFOS has

#### Read more



## Similar Compounds Simple cheminformatics search





## Relationships in the data Manual curation and mapping



A



-

## Markush Chemical representations

#### • PFOS is a member of linear perfluoroalkyl sulfonates

Perfluoroalkyl sulfonates NOCAS\_892979 | DTXSID70892979 Searched by DSSTox Substance Id.



15

ronmental Protection

## ...and their Markush Children...



• Linear perfluoroalkyl sulfonates has children...





# **Bioactivity Data**







#### ToxCast Chemical Landscape: Paving the Road to 21st Century Toxicology

Ann M. Richard<sup>\*†</sup>, Richard S. Judson<sup>†</sup>, Keith A. Houck<sup>†</sup>, Christopher M. Grulke<sup>†</sup>, Patra Volarath<sup>‡</sup>, Inthirany Thillainadarajah<sup>§</sup>, Chihae Yang<sup>∥⊥</sup>, James Rathman<sup>⊥#</sup>, Matthew T. Martin<sup>†</sup>, John F. Wambaugh<sup>†</sup>, Thomas B. Knudsen<sup>†</sup>, Jayaram Kancherla<sup>⊽</sup>, Kamel Mansouri<sup>⊽</sup>, Grace Patlewicz<sup>†</sup>, Antony J. Williams<sup>†</sup>, Stephen B. Little<sup>†</sup>, Kevin M. Crofton<sup>†</sup>, and Russell S. Thomas<sup>†</sup>

#### View Author Information $\sim$

Cite this: Chem. Res. Toxicol. 2016, 29, 8, 1225-	Article Views
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Publication Date: July 1, 2016 🗸	000/
https://doi.org/10.1021/acs.chemrestox.6b00135	LEARN

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### ToxCast/Tox21 Data





## Full transparency in terms of data



#### Concentration Response data

#### Concentration Response Data

Analytical Data on Tox21 Browser 🗹

🛃 EXPORT 👻

	Name 1	=	Description	=	Endpoint Name	=	Active	≡ Det	ta	Rep	All P	Gene	=	Intended Target	≡	Cell Line $\equiv$	Cell For	
		$\nabla$		$\nabla$		$\nabla$		$\nabla$					$\nabla$		$\nabla$			$\nabla$
	ASSAY SOURCE: ACEA		ACEA Biosciences		ACEA_AR_agonist_80hr		Inactive	ľ		~	⊞	AR		steroidal		prostate	cell line	
	ASSAY SOURCE: ACEA		ACEA Biosciences		ACEA_AR_agonist_AUC_viability		Active	ľ		~	⊞	null		cytotoxicity		prostate	cell line	
	ASSAY SOURCE: ACEA		ACEA Biosciences		ACEA_AR_antagonist_80hr		Active	ľ		₩.	⊞	AR		steroidal		prostate	cell line	
	ASSAY SOURCE: ACEA		ACEA Biosciences		ACEA_AR_antagonist_AUC_viability		Active	Ľ		₩.	⊞	null		cytotoxicity		prostate	cell line	
	ASSAY SOURCE: ACEA		ACEA Biosciences		ACEA_ER_80hr		Active	Ľ		~	⊞	ESR1		steroidal		breast	cell line	
	ASSAY SOURCE: ACEA		ACEA Biosciences		ACEA_ER_AUC_viability		Inactive	Ľ		₩.	⊞	null		cytotoxicity		breast	cell line	
	ASSAY SOURCE: APR		Apredica		APR_HepG2_CellCycleArrest_1h_dn		Inactive	Ľ			⊞	null		proliferation		liver	cell line	
	ASSAY SOURCE: APR		Apredica		APR_HepG2_CellCycleArrest_1h_up		Inactive	Ľ		.~	⊞	null		arrest		liver	cell line	
	ASSAY SOURCE: APR		Apredica		APR_HepG2_CellCycleArrest_24h_dn	n	Inactive	Ľ		.~	⊞	null		proliferation		liver	cell line	
	ASSAY SOURCE: APR		Apredica		APR_HepG2_CellCycleArrest_24h_up	)	Inactive	Ľ		~	⊞	null		arrest		liver	cell line	
	ASSAY SOURCE: APR		Apredica		APR_HepG2_CellCycleArrest_72h_dn	1	Inactive	Ľ		₩.	⊞	null		proliferation		liver	cell line	
	ASSAY SOURCE: APR		Apredica		APR_HepG2_CellCycleArrest_72h_up	)	Inactive	Ľ		₩.	⊞	null		arrest		liver	cell line	
	ASSAY SOURCE: APR		Apredica		APR_HepG2_CellLoss_1h_dn		Inactive	ľ		₩.	⊞	null		cytotoxicity		liver	cell line	
	ASSAY SOURCE: APR		Apredica		APR_HepG2_CellLoss_1h_up		Inactive	Ľ		.~	⊞	null		proliferation		liver	cell line	-
																		•
Rov	vs: 1,398							Total Row	/s: <b>1,3</b> 9	98								

## Full access to concentration-response curves





## Use Models Derived from the Data



#### Screening Chemicals for Estrogen Receptor Bioactivity Using a Computational Model

Patience Browne<sup>\*†</sup>, Richard S. Judson<sup>‡</sup>, Warren M. Casey<sup>§</sup>, Nicole C. Kleinstreuer<sup>II</sup>, and Russell S. Thomas<sup>‡</sup>

#### View Author Information $^{\sim}$

 Cite this: Environ. Sci. Technol. 2015, 49, 14, 8804– 8814
 Publication Date: June 12, 2015 ~ https://doi.org/10.1021/acs.est.5b02641 Article Views Altmetric Citations 3796 27 157



Add to Export

RIS

(\*\*)

#### Vol. 124, No. 7 | Research

#### CERAPP: Collaborative Estrogen Receptor Activity Prediction Project

Kamel Mansouri, Ahmed Abdelaziz, Aleksandra Rybacka, Alessandra Roncaglioni, Alexander Tropsha, Alexandre Varnek, Alexey Zakharov, Andrew Worth, Ann M. Richard, Christopher M. Grulke, Daniela Trisciuzzi, Denis Fourches, Dragos Horvath, Emilio Benfenati, Eugene Muratov, Eva Bay Wedebye, Francesca Grisoni, Giuseppe F. Mangiatordi, <u>... See all authors</u> V

Published: 1 July 2016 | https://doi.org/10.1289/ehp.1510267 | Cited by: 76

#### Development and Validation of a Computational Model for Androgen Receptor Activity

Nicole C. Kleinstreuer<sup>\*†</sup>, Patricia Ceger<sup>‡</sup>, Eric D. Watt<sup>§</sup>, Matthew Martin<sup>§</sup>, Keith Houck<sup>§</sup>, Patience Browne<sup>II</sup>, Russell S. Thomas<sup>§</sup>, Warren M. Casey<sup>†</sup>, David J. Dix<sup>⊥</sup>, David Allen<sup>‡</sup>, Srilatha Sakamuru<sup>#</sup>, Menghang Xia<sup>#</sup>, Ruili Huang<sup>#</sup>, and Richard Judson<sup>§</sup>

#### View Author Information $^{\sim}$

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#### Vol. 128, No. 2 | Research

#### CoMPARA: Collaborative Modeling Project for Androgen Receptor Activity

Kamel Mansouri 🔄, Nicole Kleinstreuer, Ahmed M. Abdelaziz, Domenico Alberga, Vinicius M. Alves, Patrik L. Andersson, Carolina H. Andrade, Fang Bai, Ilya Balabin, Davide Ballabio, Emilio Benfenati, Barun Bhhatarai, Scott Boyer, Jingwen Chen, Viviana Consonni, Sherif Farag, Denis Fourches, Alfonso T. García-Sosa, Paola Gramatica, Francesca Grisoni, ... <u>See all authors</u>

Published: 7 February 2020 | CID: 027002 | https://doi.org/10.1289/EHP5580 | Cited by: 2



## Searching Literature and the Internet

## Literature Searching



#### Literature - PubMed Abstract Sifter

#### Abstract Sifter Instructions

Hazard Choose Query Term Hazard Fate and Transport Metabolism/PK/PD Chemical Properties Exposure Mixtures Male Reproduction Androgen Disruption Female Reproduction GeneTox Cancer Clinical Trials Embryo and embryonic development Child (infant through adolescent) Dust and Exposure Food and Exposure Food and Exposure Water and Exposure Algae Disaster / Emergency	<ol> <li>Select PubMed starting point query</li> </ol>
Choose Query Term Hazard Fate and Transport Metabolism/PK/PD Chemical Properties Exposure Mixtures Male Reproduction Androgen Disruption Female Reproduction GeneTox Cancer Clinical Trials Embryo and embryonic development Child (infant through adolescent) Dust and Exposure Food and Exposure Water and Exposure Algae Disaster / Emergency	Hazard 🗸 🗸
HazardFate and TransportMetabolism/PK/PDChemical PropertiesExposureMixturesMale ReproductionAndrogen DisruptionFemale ReproductionGeneToxCancerClinical TrialsEmbryo and embryonic developmentChild (infant through adolescent)Dust and ExposureFood and ExposureVater and ExposureAlgaeDisaster / Emergency	Choose Query Term
Fate and Transport Metabolism/PK/PD Chemical Properties Exposure Mixtures Male Reproduction Androgen Disruption Female Reproduction GeneTox Cancer Clinical Trials Embryo and embryonic development Child (infant through adolescent) Dust and Exposure Food and Exposure Water and Exposure Algae Disaster / Emergency	Hazard
Metabolism/PK/PD Chemical Properties Exposure Mixtures Male Reproduction Androgen Disruption Female Reproduction Gene Tox Cancer Clinical Trials Embryo and embryonic development Child (infant through adolescent) Dust and Exposure Food and Exposure Food and Exposure Water and Exposure Algae Disaster / Emergency	Fate and Transport
Chemical Properties Exposure Mixtures Male Reproduction Androgen Disruption Female Reproduction GeneTox Cancer Clinical Trials Embryo and embryonic development Child (infant through adolescent) Dust and Exposure Food and Exposure Water and Exposure Algae Disaster / Emergency	Metabolism/PK/PD
Exposure Mixtures Male Reproduction Androgen Disruption Female Reproduction GeneTox Cancer Clinical Trials Embryo and embryonic development Child (infant through adolescent) Dust and Exposure Food and Exposure Water and Exposure Algae Disaster / Emergency	Chemical Properties
Mixtures Male Reproduction Androgen Disruption Female Reproduction GeneTox Cancer Clinical Trials Embryo and embryonic development Child (infant through adolescent) Dust and Exposure Food and Exposure Water and Exposure Algae Disaster / Emergency	Exposure
Male Reproduction Androgen Disruption Female Reproduction GeneTox Cancer Clinical Trials Embryo and embryonic development Child (infant through adolescent) Dust and Exposure Food and Exposure Water and Exposure Algae Disaster / Emergency	Mixtures
Androgen Disruption Female Reproduction GeneTox Cancer Clinical Trials Embryo and embryonic development Child (infant through adolescent) Dust and Exposure Food and Exposure Water and Exposure Algae Disaster / Emergency	Male Reproduction
Female Reproduction GeneTox Cancer Clinical Trials Embryo and embryonic development Child (infant through adolescent) Dust and Exposure Food and Exposure Water and Exposure Algae Disaster / Emergency	Androgen Disruption
GeneTox Cancer Clinical Trials Embryo and embryonic development Child (infant through adolescent) Dust and Exposure Food and Exposure Water and Exposure Algae Disaster / Emergency	Female Reproduction
Cancer Clinical Trials Embryo and embryonic development Child (infant through adolescent) Dust and Exposure Food and Exposure Water and Exposure Algae Disaster / Emergency	GeneTox
Clinical Trials Embryo and embryonic development Child (infant through adolescent) Dust and Exposure Food and Exposure Water and Exposure Algae Disaster / Emergency	Cancer
Embryo and embryonic development Child (infant through adolescent) Dust and Exposure Food and Exposure Water and Exposure Algae Disaster / Emergency	Clinical Trials
Child (infant through adolescent) Dust and Exposure Food and Exposure Water and Exposure Algae Disaster / Emergency	Embryo and embryonic development
Dust and Exposure Food and Exposure Water and Exposure Algae Disaster / Emergency	Child (infant through adolescent)
Food and Exposure Water and Exposure Algae Disaster / Emergency	Dust and Exposure
Water and Exposure Algae Disaster / Emergency	Food and Exposure
Algae Disaster / Emergency	Water and Exposure
Disaster / Emergency	Algae
· · ·	Disaster / Emergency

Optionally, enter any PubMed query or edit the query from step 1 ("50-32-8" OR "Benzo(a)pyrene") AND (NOAEL OR NOEL OR LOEL OR Rfd OR "reference dose" OR "reference concentration" OR "adverse effect level"[tiab] OR "cancer slope factor"[tiab])



- Real-time retrieval of data from PubMed ~30 million abstracts and growing)
- Choose from set of pre-defined queries
- Adjust and fine tune queries based on interests

## Literature Searching



- "Sifting" of results using multiple terms
- Frequency counting terms
- Color highlighting of terms
- Download list to Excel
- Send list to PubMed for downloading ref. file
- Direct link via PubMed ID

Abotidut		5115											
1 Select P	ubMed starting poir	nt query			2 Optiona	lly, edit the query before retrieving.			3 Click Retrieve Artic	es to begin download.	Option	onally, expor	t articles
Hazard				~	("80-05-7 "reference [tiab] OR '	OR "Bisphenol A") AND (NOAEL Of e dose" OR "reference concentration cancer slope factor"[tiab])	≷ NOEL OR L( n" OR "advers	OEL OR Rfd OR se effect level" //	RETRIEVE ARTICLES	ded	🛓 SENI	010 -	
find articles	quickly, enter terms	to sift abstra	acts.										
strogen	Bisphenol												
trogen ↓	Bisphenol ↓↑	T ↓↑	- F	PubMe	Y ↓↑	Title ↓↑	=	Authors ↓↑	=	Journal ↓↑	≡	Rev ↓↑	DOI ↓↑
							V		$\nabla$		$\nabla$		
	4	6		34147626	2021	Modulation of Folliculogenesis in Adu	It Laying	Eldefrawy; Xu; Pusch; K	arkoura; Alsafy; Elgendy;	Reproductive toxicology (Elmsford, N.Y.)			10.1016/j.rep
	9	9		34146661	2021	Effects of bisphenols on Blood-Testis B	3arrier pro	Peña-Corona; Vásquez	: Aguire; Vargas; Juárez;	Reproductive toxicology (Elmsford, N.Y.)		$\checkmark$	10.1016/j.rep
	2	5		33802611	2021	Characterization of Estrogenic Activity	and Site	Chioccarelli; Migliaccio	; Suglia; Manfrevola; Porr	International journal of molecular sciences			10.3390/ijm
	2	2		3666848	2021	A comprehensive review on the carcir	nogenic p	Khan; Correia; Adiga; F	lai; Dsouza; Chakrabarty;	Environmental science and pollution resea	rch in	$\checkmark$	10.1007/s113
	2	2		3640550	2021	A reconnaissance study of pharmaceu	uticals, pes	Picó; Campo; Alfarhan;	El-Sheikh; Barceló	The Science of the total environment			10.1016/j.sci
	2	2		3516155	2021	Update on the Health Effects of Bisph	enol A: O	Vom Saal; Vandenberg		Endocrinology			10.1210/end
	2	2		3212759	2020	Gestational Exposure to Bisphenol A A	Affects Test	Karmakar; Ahn; Kim; Ju	ing; Kim; Lee; Ryu	International journal of molecular sciences			10.3390/ijm
	2	4		3010594	2020	Effects of bisphenol A at the safe refe	rence dos	Li; Gao; Tan; Miao; Fan;	Gao; Liu; Ding; Shi; Song	Ecotoxicology and environmental safety			10.1016/j.ecc
	9	11		3010167	2020	Bisphenol AF and Bisphenol F Induce	Similar Fe	Mentor; Wänn; Brunstr	öm; Jönsson; Mattsson	Toxicological sciences : an official journal o	f the		10.1093/toxs

## What's the best way to search the internet for chemical data?



- We know how complex chemicals identifiers are...
  - CASRN(s)
  - Hundreds of names (maybe)
  - SMILES
  - InChIs
  - EINECS, EC numbers
- What can WE do to help you navigate the internet?

## External Links – Also use Identifiers Names, CASRN, PubChem IDs, InChIs



Benzo(a)pyrene 50-32-8 | DTXSID2020139

Searched by DSSTox Substance Id.

General

EPA Substance Registry Service

PubChem

Chemspider

CPCat

🥖 DrugBank

W Wikipedia

Q MSDS Lookup

ChEMBL

😨 ToxPlanet

ACS Reagent Chemicals

🜞 Wolfram Alpha

🔀 ECHA Infocard

🖳 ChemAgora

Consumer Product Information Database

ChEBI

NIST Chemistry Webbook

WEBWISER

PubChem Safety Sheet

PubChem: Chemical Vendors

Consumer Product Information Database

Toxicology

ACToR

on DrugPortal

CCRIS

ChemView

CTD

Gene-Tox

HSDB

ACToR PDF Report

CREST

ECOTOX

ChemView

BindinaDB

Chemical Checker

MIOSH IDLH Values

actMed

ECOTOX

Publications

and Toxline

PPRTVWEB

🕪 PubMed

IRIS Assessments

🖲 EPA HERO

NIOSH Skin Notation Profiles

🗰 NIOSH Pocket Guide

RSC Publications

🕌 BioCaddie DataMed

 Springer Materials

Bielefeld Academic Search Engine

CORE Literature Search

G Google Books (Text Search)

Google Patents (Text search)

Google Scholar (Text search)

G Google Patents (Structure search)

G Google Books (Structure Search)

Google Scholar (Structure search)

Federal Register

#### Analytical

RSC Analytical Abstracts

🗟 Tox21 Analytical Data

MONA: MassBank North America

imzCloud 🌰

NIST IR Spectrum

NIST MS Spectrum

🛋 MassBank

NIST Antoine Constants

IR Spectra on PubChem

NIST Kovats Index values

Protein DataBank

🍐 National Environmental Methods Index

#### Prediction

2D NMR HSQC/HMBC Prediction

Carbon-13 NMR Prediction

Proton NMR Prediction

\* ChemRTP Predictor

LSERD

SEPA United States Environmental Protection

## External Links



#### Links to ~90 websites providing access to additional data on the chemical of interest



						Print 😝 Eng	glish 🗸
eChem	Portal			Th Che	e Globa Infor mical S	al Portal mation o ubstanc	to on es
Home Substance Search Property Search	Classification Search	Schedules of Assessments	Data sources	About 🕶	Help 🕶	Contact Us	
b Chemical Substance	Search						
Substance (50-32-8)							~
Sources and type of information							^
Select all Deselect all							
Types ③	Data sources						
Property information	ACToR <sup>0</sup>	AGRITO>	Ø		CIS assessme	ents	
Exposure and use information	APVMA-CR	CCR •		CI	ESAR <sup>0</sup>		
GHS classifications	Chemicals Dashboa	ard <sup>10</sup> ChemInf	0	<b>C</b>	ombined Exp	osures <sup>(1)</sup>	



# Chemical Lists and Categories

#### A List of Lists of Chemicals

https://comptox.epa.gov/dashboard/chemical\_lists



Q Search Chemi	ical Lists				LEXPORT - CD COPY URL
				Showi	ng 36 of 319 Records
List Acronym 🖓	$\equiv \mid$ List Name		# Chemicals	Updated	List Description
PFAS		V			
EPAPFASDW537	PFAS EPA WATER: Existing	EPA DW Method	19	2019-11-16	EPA has recently revised method 537.1 for the PFAS on this list to detect them in drinking water.
EPAPFASDWTREAT	PFAS EPA WATER: Drinking	Water Treatment	9	2019-11-16	EPA is gathering and evaluating treatment effectiveness and cost data for removing these PFAS from drinking water systems.
EPAPFASINSOL	PFAS EPA: Chemical Inven	ory Insoluble in	43	2021-11-21	Per- and Polyfluoroalkyl Substances (PFASs) in EPA's expanded ToxCast chemical inventory that were determined to be insoluble in DMSO above 5mM concentration. These PFAS chemicals were successfully procured from commercial suppliers (with a small number provided by National Toxicology Program partners) but deemed unsuitable for testing due to limited DMSO solubility. For a complete list of solubilized PFAS in EPA's inventory, see https://comptox.epa.gov/dashboard/chemical-lists/EPAPFASINV
EPAPFASINV	PFAS EPA: ToxCast Chemic	al Inventory	430	2021-11-21	Per- and Polyfluoroalkyl Substances (PFAS) included in EPA's expanded ToxCast chemical inventory and available for testing. These PFAS chemicals were successfully procured from commercial suppliers (with a small number provided by National Toxicology Program partners) and were deemed suitable for testing (i.e., solubilized in DMSO above 5mM, and not gaseous or highly reactive). All or portions of this inventory are being made available to EPA researchers and collaborators to be analyzed and tested in various high-throughput screening (HTS) and high-throughput toxicity (HTT) assays.
	,	,			The https://comptox.epa.gov/dashboard/chemical-lists/EPAPFAS75S1 list is a prioritized subset of this larger chemical inventory.

#### The OECD List of PFAS

http://www.oecd.org/chemicalsafety/portal-perfluorinated-chemicals/

#### PFAS: Listed in OECD Global Database

Search for chemical by systematic name, synonym, CAS number, DTXSID or InChIKey

Identifier substring search

#### List Details

Description: OECD released a New Comprehensive Global Database of Per- and Polyfluoroalkyl Substances (PFASs) listing more than 4700 new PFAS, including several new groups of PFASs that fulfill the common definition of PFASs (i.e. they contain at least one perfluoroalkyl moiety) but have not yet been commonly regarded as PFASs. The list can be used in conjunction with the methodology report summarising the major findings with respect to the total numbers and types of PFASs identified, the limitations, gaps and challenges identified, and opportunities for improving the future understanding of PFASs production, use on the global market, and presence in the environment, biota, and other matrices.

#### Source website: http://www.oecd.org/chemicalsafety/portal-perfluorinated-chemicals

A major effort was undertaken to register this list within DSSTox, adding chemical structures for as many PFAS entries as possible using both manual and auto-mapping (structures using CAS-matching) curation methods. The result is that approximately 1/3 of the list is curated at the highest two curation levels (DSSTox\_High or DSSTox\_Low) currently, whereas more than half of this list is registered at the Public\_Low curation level (based on PubChem content). The PFASOECD list is undergoing continuous registration and curation.

Number of Chemicals: 4729





✓ Q

## Example PFAS-UVCBs





Ethene, tetrafluoro-, oxidized, polymd., reduced, decarboxylated, C6 fraction 274917-96-3 | DTXSID00108075

1-Propene, 1,1,2,3,3,3-hexafluoro-, polymer with 1,1-difluoroethene, ethene, 1,1,2,2tetrafluoroethene and 1,1,2-trifluoro-2-(trifluoromethoxy)ethene 149935-01-3 | DTXSID00108732

#### PFAS List Paper https://doi.org/10.3389/fenvs.2022.850019





#### Assembly and Curation of Lists of Per- and Polyfluoroalkyl Substances (PFAS) to Support Environmental Science Research

Antony J. Williams<sup>1\*</sup>, Linda G. T. Gaines<sup>2</sup>, Christopher M. Grulke<sup>1†</sup>, Charles N. Lowe<sup>1</sup>, Gabriel F. B. Sinclair<sup>3</sup>, Vicente Samano<sup>4</sup>, Inthirany Thillainadarajah<sup>4</sup>, Bryan Meyer<sup>4</sup>, Grace Patlewicz<sup>1</sup> and Ann M. Richard<sup>1</sup>

- What makes our efforts different?
- MANUAL curation work
- Building lists, crossreferencing, mapping relationships, sourcing and curating data



## **Batch Searching**

#### **Batch Searching**



- Singleton searches are great but...
- ...we generally want data on LOTS of chemicals!
- Typical questions
  - What are the structures for a set of chemical names? Set of CASRNs?
  - Can I get chemical lists in Excel files? As a list of SMILES strings? Can I get an SDF file?
  - Can I include predicted properties? OPERA? TEST?
  - Are "these chemicals" screened in Toxcast?
  - I need masses and formulae for a list of chemicals

## Batch Search



Batch Sear	ch		
Select Input Type	e(s)	2 Enter Identifiers to Sea	arch
Substance Ider	ntifiers Name	(Please enter one identifier per line.	e. Processing time increases with number of inputs.)
CASRN	INdifie	DTXSID9020374	A
InChIKey		DTXSID9020827	
DSSTox S	Substance ID	DTXSID2022678	
DSSTox Comp	ound ID	DTXSID4023381	
InChIKey Skele	ton	DTXSID7032004	
MS-Ready Forr	nula(e)	DTXSID4022361	
Exact Formula	(e)	DTXSID8021771	
	VId55	3 OISPLAY ALL CHEMICALS	LS OF CHOOSE EXPORT OPTIONS
	45% loaded		
		45 Chemicals Found from 110 Input(s)	
REPLACE IDENTIFIERS V	VITH SELECTED CHEMICALS		
Structure	DTXSID		$\equiv$ Mono. Mass $\equiv$ Mol. Formula $\equiv$
		Σ	
	DTXSID2022678 Bicalutamide	90357-06-5	5 430.061041 <u>C18H14F4N2O4S</u>
° Corretto	DTXSID3020621		

## Batch Search – Excel, CSV, SDF file





#### Presence in Lists

Description

V

Download Export file for the chemicals selected

**DOWNLOAD EXPORT FILE** 

5

#### Batch Search



AutoSave 💽 🖪 🥠 🗸 🖓 🗸 😴	CCD-Batch-Search_2022-03-27_	05_36_52.xlsx 👻 🔎	Search		Williams, Anton	y 🚾 🖬	- 0	×
File Home Insert Draw Page La	ayout Formulas Data I	Review View Deve	eloper Help			🖻 Share	🖓 Comr	ments
$\begin{array}{c c} & & \\ & &$	A <sup>×</sup> ≡ ≡ ≡ ≫ × ab Wra × ≡ ≡ ≡ ≡ Ξ ⊡ Æ Me	ap Text General General rge & Center • \$ • \$	% 9 ←0 .00 .00 →0 Condi Format	tional Format as Cell tting ~ Table ~ Styles ~	Insert ~     ∑       Insert ~     ↓       Delete ~     ↓       Format ~     ♦	→ A ZZ → O Sort & Find & Filter → Select →	Sensitivity	
Clipboard 🔽 Font	د Alignment	N N	lumber 🔽	Styles	Cells	Editing	Sensitivity	^
A2 · : × $\checkmark$ $f_x$ DTXS	ID9020299							~
AB	C D E	F	G H	I J	K L	M N	0	P
1 DTXSID PREFERRED_NAME	INCHIKEY CASRN SMILES	MOLECULAR_FORMULA	AVERAGE_MONOISOS	AFETY_D DATA_SOUN	JMBER_IRIS_LINK AT	MOSPH BIOCONCE	3IODEGRAB	
2 DTXSID9020299 Chlorobenzilate	RAPBNVD: 510-15-6 CCOC(=O)	C16H14Cl2O3	325.19 324.032	154	16 Y 1.3	37E-11 477.542	4.6243	349.9
3 DTXSID6034712 Mesosulfuron-methyl	NIFKBBMC 208465-21COC(=O)C	C17H21N5O9S2	503.5 503.0781	/ 95	10 1.	79E-11 3.2453	4.26547	254.0
4 DTXSID7034753 Foramsulfuron	PXDNXJSD 173159-57 COC1=CC	C17H20N6O7S	452.44 452.1114	/ 95	2.5	35E-11 3.84639	5.67465	265.1
5 DTXSID1033664 17-Methyltestosterone	GCKMFJBC58-18-4 C[C@]1(O	C20H30O2	302.458 302.2246	/ 145	1377 3.	99E-11 62.2298	97.9166	294.8
6 DTXSID8034401 Buprofezin	PRLVTUNV 69327-76- CC(C)N1C	(C16H23N3OS	305.44 305.1562	/ 134	42 1.3	38E-11 52.49	6.89035	353.7
7 DTXSID0020529 2,4-Dinitrotoluene	RMBFBMJ 121-14-2 CC1=C(C=	(C7H6N2O4	182.135 182.0328 Y	/ 198	379 Y 1.	63E-12 9.12436	3.5609	299.8
8 DTXSID2034673 Iodosulfuron methyl ester	r JUJFQMPK 144550-36 [Na+].COC	C14H13IN5NaO6S	529.24 528.9529 Y	/ 88	1.	77E-11 3.51252	4.73647	265.0
9 DTXSID7024247 Pentachlorobenzene	CEOCDNV 608-93-5 CIC1=CC(C	C6HCl5	250.32 247.8521	/ 170	84 Y 2.1	25E-13 5620.75	6.16855	277.0
10 DTXSID0034227 Icaridin	QLHULAH(119515-38 CCC(C)OC	C12H23NO3	229.32 229.1678	/ 111	67 1.	32E-11 3.81105	5.17405	251.8
11 DTXSID0020440 Dichlorprop	MZHCENG 120-36-5 CC(OC1=C	C9H8Cl2O3	235.06 233.985	164	89 1.	16E-11 3.54397	3.53597	298.4
12 DTXSID9034816 Monocrotophos	KRTSDMXI 6923-22-4 CNC(=O)\	(C7H14NO5P	223.165 223.061	152	274 2.	77E-11 0.922318	4.13837	301.7
13 DTXSID8021301 Tamoxifen citrate	FQZYTYWI54965-24- OC(=O)CC	C32H37NO8	563.647 563.2519	/ 90	17257 2	9E-11 1209.93	3.36316	419.3
14 DTXSID7032553 Flumetralin	PWNAWO 62924-70- CCN(CC1=	C16H12ClF4N3O4	421.73 421.0452	/ 117	1.3	38E-11 35265.1	3.54617	347.7
15 DTXSID6024048 Difenzoquat metilsulfate	XQEMNBN 43222-48- COS([O-])	(C18H20N2O4S	360.43 360.1144	79	20 <mark>Y</mark> 1.9	93E-11 565.107	13.7793	335
16 DTXSID3024104 Fluoranthene	GVEPBJHC 206-44-0 C1=CC2=C	C16H10	202.256 202.0783	211	398 Y 4.	98E-11 3528.4	147.199	393.9
17 DTXSID8023890 Asulam	VGPYEHKC 3337-71-1 COC(=O)N	C8H10N2O4S	230.24 230.0361	/ 133	19 <mark>Y</mark> 1.3	21E-11 2.50573	4.63676	254.8
18 DTXSID4032532 Carfentrazone-ethyl	MLKCGVH 128639-02 CCOC(=O)	C15H14Cl2F3N3O3	412.19 411.0364	/ 133	9 2.	16E-11 192.141	4.88739	352.4
19 DTXSID5032498 Triclosan	XEFQLINVI 3380-34-5 OC1=C(OC	C12H7Cl3O2	289.54 287.9512	246	2221 1.	74E-11 52.8927	4.50619	342.3
20 DTXSID1021160 Picloram	NQQVFXU 1918-02-1 NC1=C(CI)	C6H3Cl3N2O2	241.45 239.926	<b>/</b> 186	133 Y 8.	15E-12 2.72427	4.09513	296.1
21 DTXSID9020160 Bifenthrin	OMFRMAI 82657-04- CC1=C(C=	(C23H22ClF3O2	422.87 422.126	( 172	246 Y 3.3	32E-11 4990.65	3.54377	370.9
Cover Sheet Main Data +	)			4			0 000 / 0	► T
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## Open Data Exchange

## Since our data are Open...



#### • They flow into other systems for benefit ...

- ECHA eChemPortal
- ChemSpider
- EBI's UniChem
- PubChem

0 Use and Man	ufacturing	?
0.1 Uses		?
PA CPDat Chemical and Pro	oduct Categories	
0 items View More 🔀		👱 Downlo
	SORT BY 🔶 Category	
Category	Category Description	Categorization Type
Construction and building naterials	Materials used for construction (e.g. flooring, tile, sinks, bathtubs, mirrors, wall materials/drywall, wall-to-wall carpets, insulation, playground su 🔤	Product Use Category (PUC)
binder		OECD Functional Use
binder		Reported Functional Us
catalyst		Reported Functional Us
epoxy hardener, curing agent		Reported Functional Use





## Developing Cheminformatics "PoC Modules"





- Hazard Comparison Profiling profile chemicals based on hazard
- Alerts structure, substructure, SMARTS based alerts and flags
- Predict batch prediction using WebTEST (100s of structures)
- Search structure/substructure/similarity searches
- Standardize convert structures into QSAR/MS-Ready forms
- ToxPrints generate ToxPrint substructural fragments and profile

## Module 1: Hazard Module



d c												🛠 наz	ARD	🖶 PR	EDICT	So S Hazar	EARCH d assessr	ی 🧐 nent prof	STAND	ARDI
				Toxicity:	VH - Ver	y High <mark>H</mark>	- High <mark>N</mark>	<mark>1</mark> - Mediu	m L - Lo	w I - Inco	onclusive N	/A - Not App	olicable	Authority:	Authorita	Full Full Custor Emerg	m Jency Re	sponse	\$	V
Skinned (6)	Acute M	lammalian	Toxicity		nicit		Human	Health E	Neuro	toxicity	Systemi	c Toxicity				Site-S	pecific S	creening	_	
<ul> <li>Skipped (6)</li> <li>Unlikely (0)</li> <li>Filters (0)</li> <li>Sorting (0)</li> <li>Structure</li> <li>CAS</li> <li>Name</li> </ul>	Oral	Inhalation	Dermal	Carcinogenicity	Genotoxicity Mutager	Endocrine Disruption	Reproductive	Developmental	Repeat Exposure	Single Exposure	Repeat Exposure	Single Exposure	Skin Sensitization	Skin Irritation	Eye Irritation	Acute Aquatic Toxicit	Chronic Aquatic Toxic	Persistence	Bioaccumulation	
60-35-5 Acetamide	L	I	T	VH	VH	L	М	М	I	I	L	I	I	Т	I	L	L	L	L	
107-13-1 Acrylonitrile	н	н	н	VH	VH	L	н	н	н	н	н	м	н	н	VH	н	н	н	L	
1912-24-9 Atrazine	М	н	L	VH	L	Н	Н	н	н	М	м		н	L	м	VH	VH	н	L	



Hazard version: U/	Comparison Dashboard AT, build: 2021-10-26 21:27:37 UTC		🖗 HAZARD \land ALERTS	🖬 PREDICT 🕄 SEARCH 🕼 STANE	DARDIZE @ TOXPRINTS
$\uparrow$	Search in any field Q			Collapse Details	
#	ID	Chemical		ashby	ttc
6	50594-66-6			♦	bond:CX_halide_alkenyl- X_dihalo_(1_2-), bond:CX_halide_alkyl- Cl_dichloro_(1_1-), bond:CX_halide_alkyl- X_dihalo_(1_3),
10	309-00-2				bond:CX_halide_generic- X_dihalo_(1_2-)
14	82-28-0			$\diamond$	♦
15	3775-55-1			<b>1</b>	<b>⊘</b> ⁰

### Module 3: WebTEST Batch Prediction





### Module 4: Structure/Substructure/Similarity





## Summary and Conclusion





- CompTox Chemicals Dashboard a central hub for environmental data
  - ~900k chemical substances (1.2M soon)
  - Integrating property data, hazard data, exposure data, *in vitro* bioactivity data
  - Interrogation of bioactivity data -
  - Multiple types of searches



- Batch search for thousands of chemicals
- Real-time property and toxicity predictions
- Downloadable files CSV, TSV and Excel

## Some Related Publications of Interest





Computational Toxicology Volume 12, November 2019, 100096



EPA's DSSTox database: History of development of a curated chemistry resource supporting computational toxicology research

Christopher M. Grulke <sup>a</sup>, Antony J. Williams <sup>a</sup>, Inthirany Thillanadarajah <sup>b</sup>, Ann M. Richard <sup>a</sup> 📯 🖾

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#### Enabling High-Throughput Searches for Multiple Chemical Data Using the U.S.-EPA CompTox Chemicals Dashboard

Charles N. Lowe\* and Antony J. Williams\*

Cite this: J. Chem. Inf. Model. 2021, 61, 2, 565–570 Publication Date: January 22, 2021 ∨ https://doi.org/10.1021/acs.jcim.0c01273 This article not subject to U.S. Copyright. Published 2021 by American Chemical Society RIGHTS & PERMISSIONS ✓ Subscribed

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#### Database | Open Access | Published: 28 November 2017

## The CompTox Chemistry Dashboard: a community data resource for environmental chemistry

Antony J. Williams <sup>CI</sup>, <u>Christopher M. Grulke</u>, Jeff Edwards, <u>Andrew D. McEachran</u>, <u>Kamel Mansouri</u>, <u>Nancy C. Baker</u>, <u>Grace Patlewicz</u>, <u>Imran Shah</u>, <u>John F. Wambaugh</u>, <u>Richard S. Judson</u> & <u>Ann M. Richard</u>

Journal of Cheminformatics 9, Article number: 61 (2017) Cite this article



Environment International Volume 154, September 2021, 106566



#### Review article

Sourcing data on chemical properties and hazard data from the US-EPA CompTox Chemicals Dashboard: A practical guide for human risk assessment

Antony J. Williams <sup>a</sup> 😤 🖾, Jason C. Lambert <sup>a</sup>, Kris Thayer <sup>b</sup>, Jean-Lou C.M. Dorne <sup>c</sup>

## You want to know more...



- Lots of resources available
  - Presentations: <u>https://tinyurl.com/w5hqs55</u>
  - Communities of Practice Videos: <u>https://rb.gy/qsbno1</u>
  - Manual: <u>https://rb.gy/4fgydc</u>
  - Latest News: <u>https://comptox.epa.gov/dashboard/news\_info</u>

Q Antony William	ns		help? 🔀
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Antony Williams, the ChermConnection: A career path through a diverse series of robs and responsibilities Amay sitilities Memory and the series of the serie	The needs for chemistry standards, database tools and data curration at the chemical-biology interface Areas titler, face Maxan de Balander Chemister	ANNOUNCEMENT EDSP21 and ToxCast Dashboards To Be Discontinued	And have a factor of the second
Antony Williams, the ChemConnector: A career path thr Intony Williams 09/05/2019	The needs for chemistry standards, database tools and data curation a Antony Williams ~ 30/06/2017	EDSP21 and ToxCast Dashboards To Be Discontinued Antory Williams 30/07/2019	Non-Targeted Screening of Wastewater for Water Reuse using Jerry Zweigenbaum ~ 12/09/2019
Investigating Report Marines for Parlomenes to the USE EPA National Center for Computational Tockslopy Mary Billion - State State State State Mark State S	Conserves anking and fragmeniation predictors for identification of manyowns in high resultion mass spectrometry and the first state of the second state of the second many states of the second state of the second states of the many states of the second states tates of the second st	Building an Online Profile Using Social Networking Tools Challed In Company of Company Unlined In Company of Company	The CompTox Chemicals Databoard as An Indegration Hub for Chemistry, Biology and Environmental Touchy Data
hvestigating Impact Metrics for Performance for the US EPA Natio 000-0002-2668-4021 - 30/06/2017	Consensus ranking and fragmentation prediction for identif Andrew McEachran ~ 21/08/2018	Building an Online Profile Using Social Networking Tools Antony Williams ~ 30/05/2018	The CompTox Chemicals Dashboard as An Integration Hub for Chemistr Antony Williams ~ 09/10/2019
AND	CECCL: COOL and in the second	The EPA Comp Tox Chemistry Dashpaser - a centralized hub for environmental scencios     August Chemistry Chemistry environmental scencios     August Chemistry     August Ch	Environmental Communy Company Memory Standards Hangabards Man Spectromory Stat Hergania to the EPA Chemistry Seabard Many J. Blanz, Auros Matatina, Are Bina, Re Mann, Er Lin, On Joa San Status, and Bina, Re
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Where are we now? Celebrating the 10th Incremental Release of the CompTox Chemicals Dashboard

#### CompTox Chemicals Dashboard primer videos

The CompTox Chemicals Dashboard is a one-stop-shop for chemistry, toxicity and exposure information for over 875,000 chemicals. Data and models within the Dashboard also help with efforts to identify chemicals of most need of further testing and reducing the use of animals in chemical testing.

Explore the wealth of data and features available in the CompTox Chemicals Dashboard with these insructional videos narrated by EPA scientists.

#### General Chemistry and Search Capabilities



## Acknowledgments



- Contact: <u>Williams.Antony@epa.gov</u>
- Feedback and follow-up is welcomed! Your questions help.
- The dashboard is based on the efforts of many more team members than us
- Many collaborators provide data also



EPA's Center for Computational Toxicology and Exposure