http://www.orcid.org/0000-0002-2668-4821

EPA United States Environmental Protection Agency

The EPA CompTox Chemicals Dashboard: A Web-Based Data Integration Hub for Environmental Chemistry and Toxicology Data

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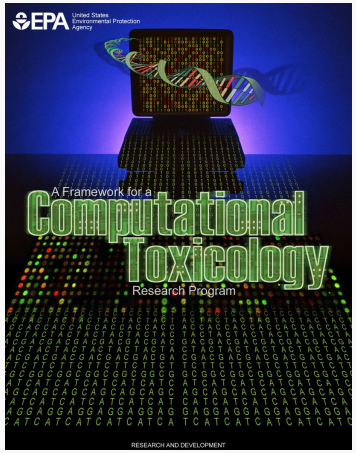
U.S. Environmental Protection Agency, RTP, NC

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

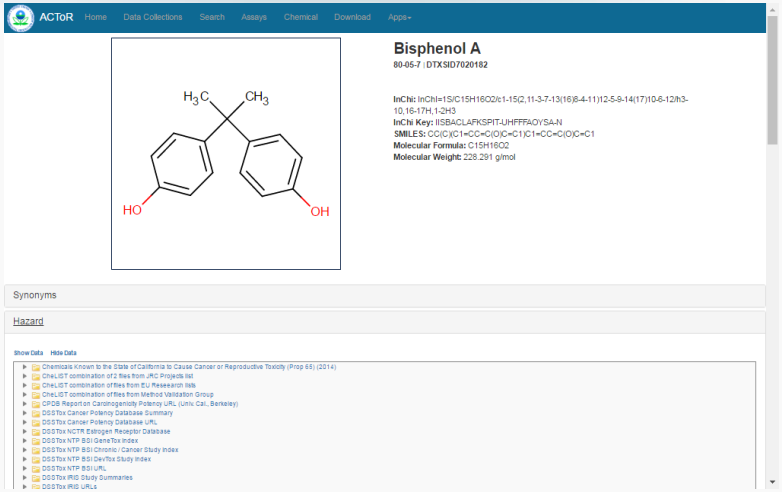
October 2nd 2018

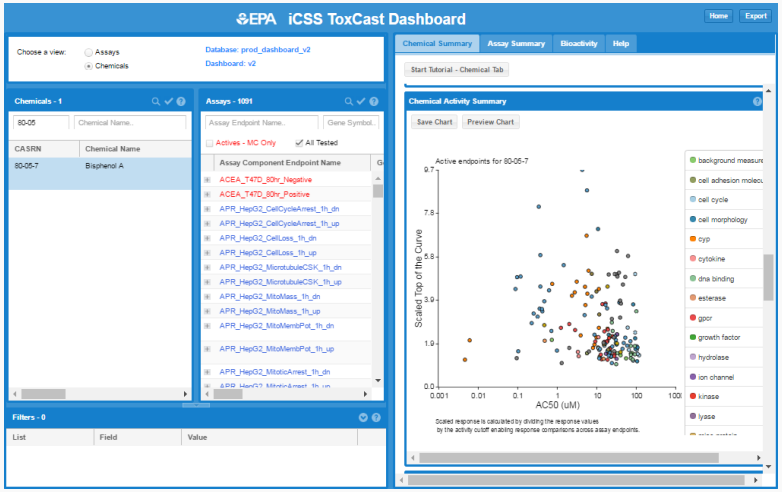
National Center for Computational Toxicology

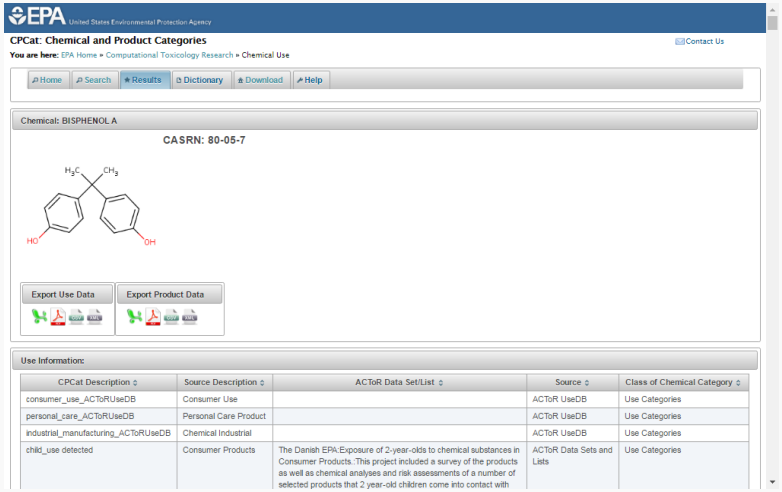


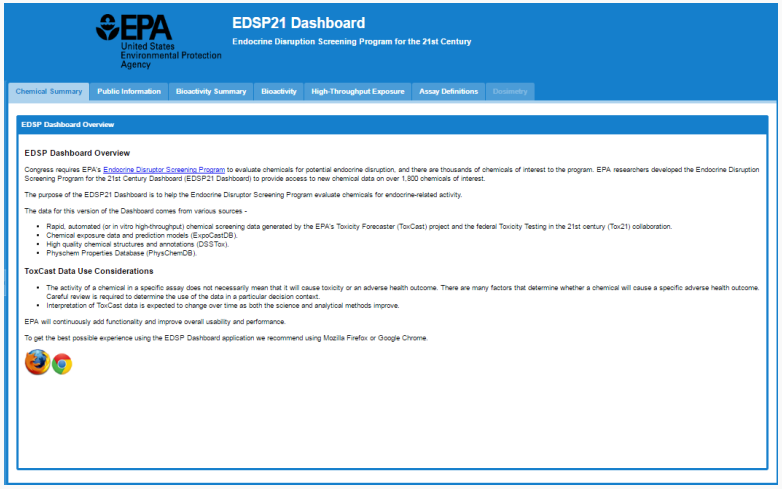
- National Center for Computational Toxicology established in 2005 to integrate:
  - High-throughput and high-content technologies
  - Modern molecular biology
  - Data mining and statistical modeling
  - Computational biology and chemistry
- Currently staffed by ~60 employees as part of EPA's Office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

Earlier Dashboard Applications







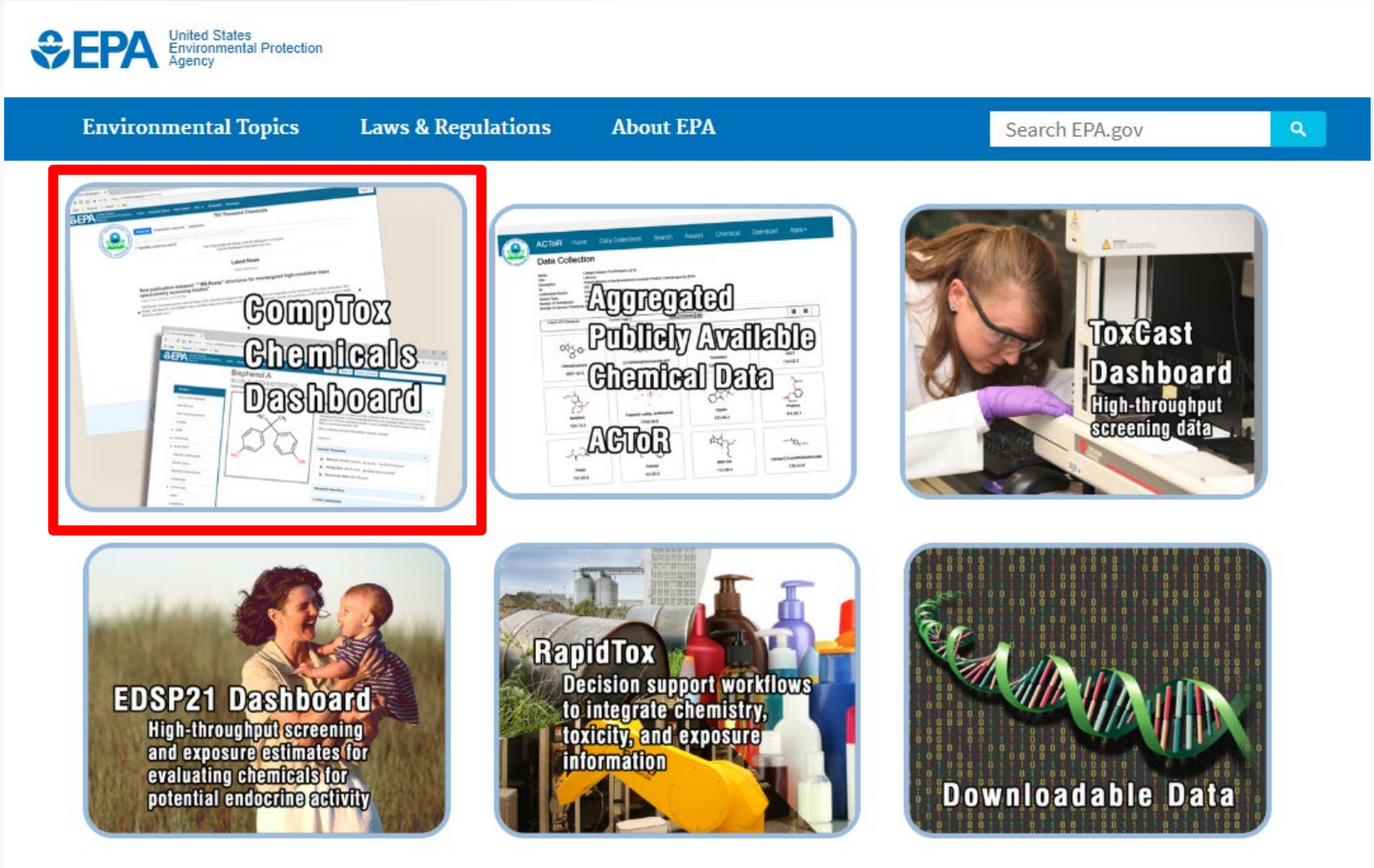


The CompTox Portal
https://comptox.epa.gov/

EPA United States Environmental Protection Agency

Environmental Topics | Laws & Regulations | About EPA | Search EPA.gov

The CompTox Portal
https://comptox.epa.gov/

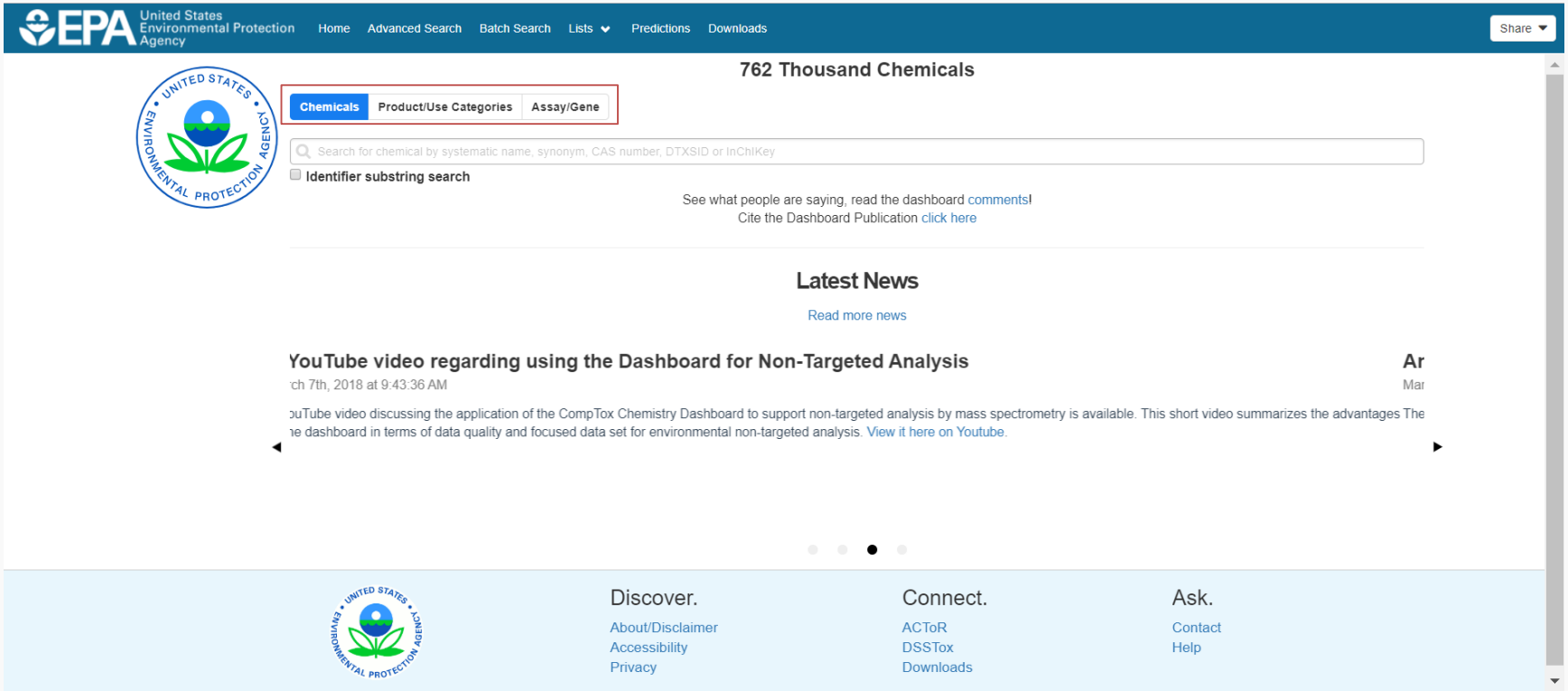


The CompTox Chemicals Dashboard

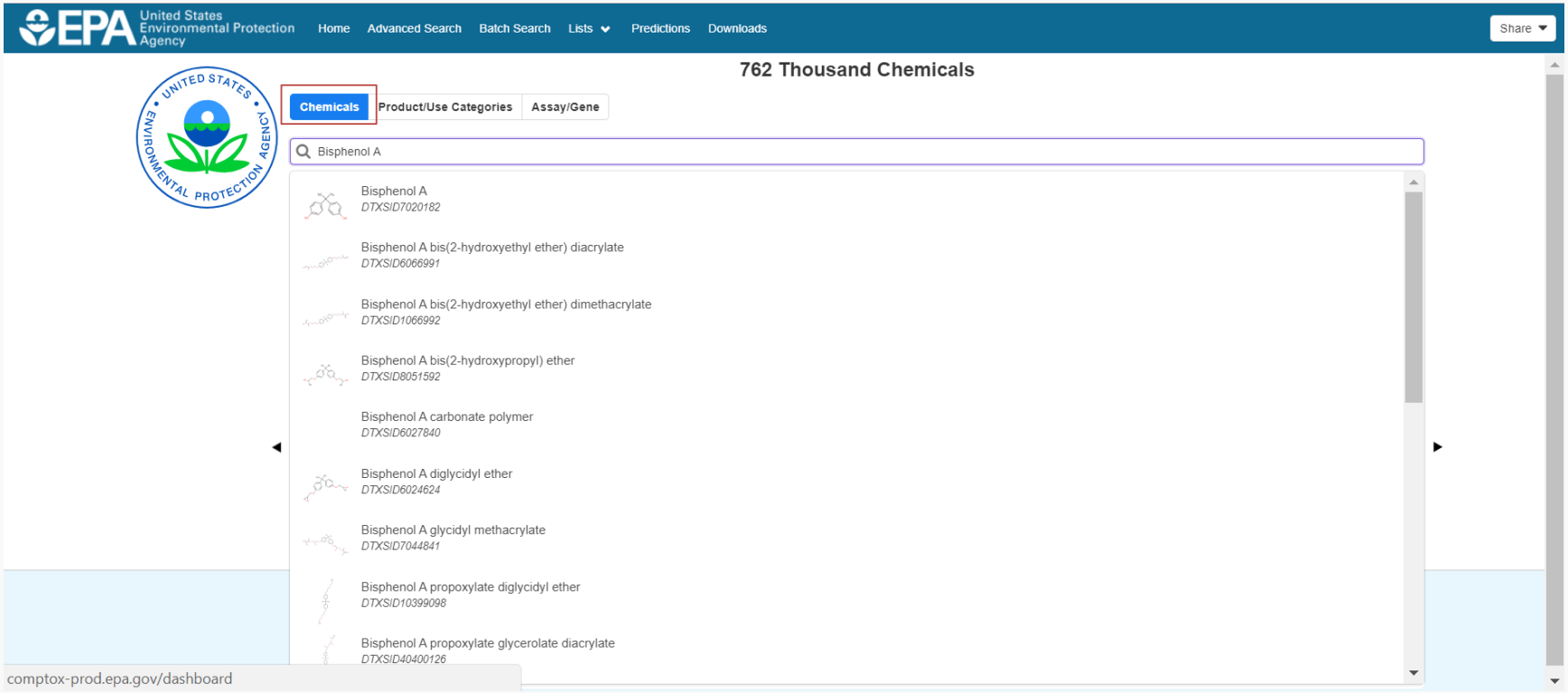
- A **publicly accessible website** delivering access:
  - ~765,000 chemicals with related property data
  - Experimental and predicted physicochemical property data
  - Integration to “biological assay data” for 1000s of chemicals
  - Information regarding consumer products containing chemicals
  - Links to other agency websites and public data resources
  - “Literature” searches for chemicals using public resources
  - “Batch searching” for thousands of chemicals
  - **DOWNLOADABLE Open Data for reuse and repurposing**

CompTox Chemicals Dashboard

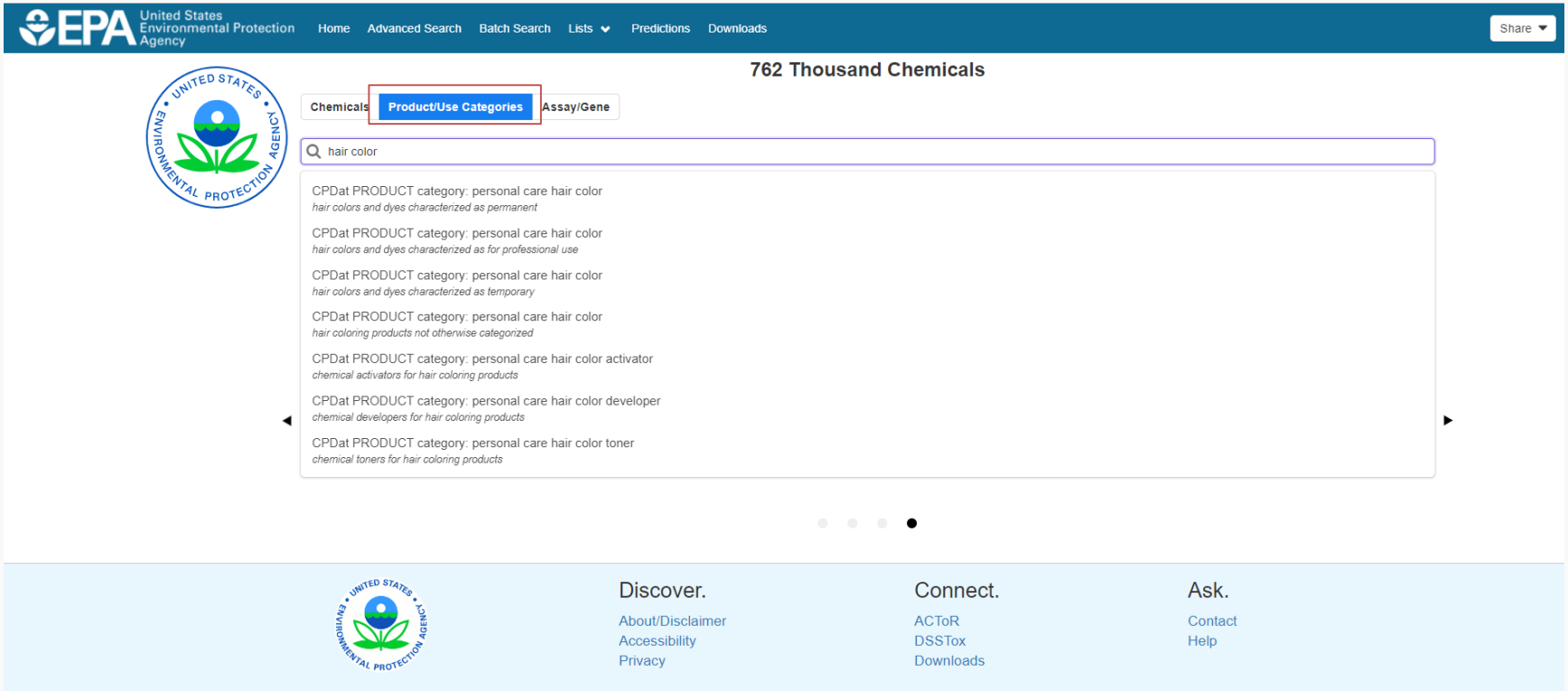
https://comptox.epa.gov/dashboard



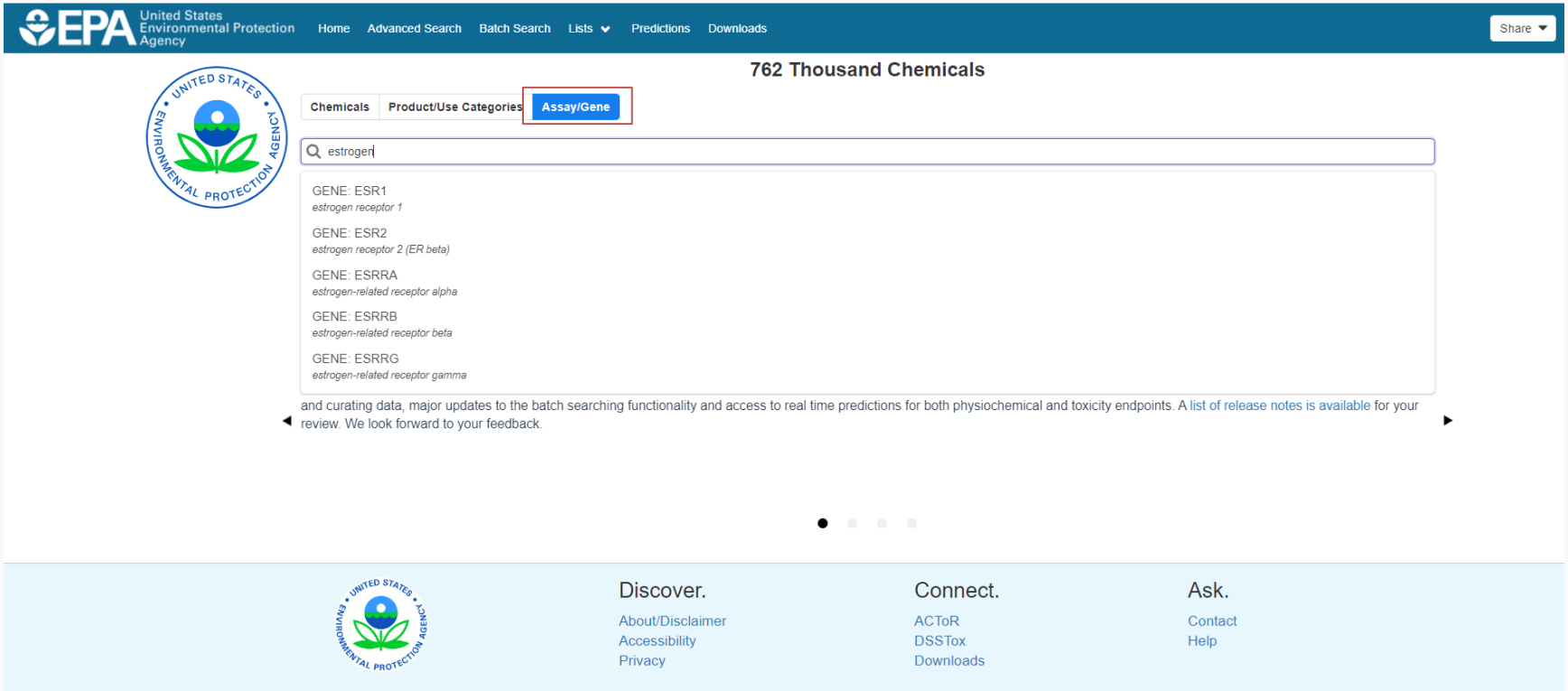
CompTox Chemicals Dashboard
Chemicals



CompTox Chemicals Dashboard
Products and Use Categories



CompTox Chemicals Dashboard
Assays and Genes



Detailed Chemical Pages

EPA United States Environmental Protection Agency

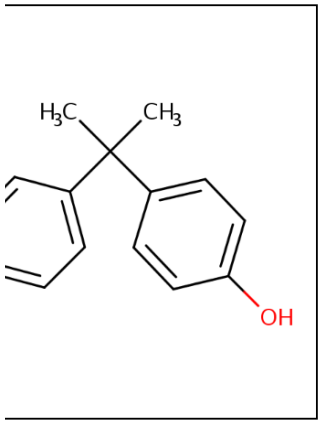
- **DETAILS**
- EXECUTIVE SUMMARY
- PROPERTIES
- ENV. FATE/TRANSPORT
- HAZARD
- ADME
- EXPOSURE
- BIOACTIVITY
- SIMILAR COMPOUNDS
- GENRA (BETA)
- RELATED SUBSTANCES
- SYNONYMS
- LITERATURE
- LINKS
- COMMENTS

h Batch Search Lists Predictions Downloads Copy Share Submit Comment Search all data

nol A

DTXSID7020182

SSTox Substance Id.



Wikipedia

Bisphenol A (**BPA**) is an organic synthetic compound with the chemical formula $(CH_3)_2C(C_6H_4OH)_2$ belonging to the group of diphenylmethane derivatives and bisphenols, with two hydroxyphenyl groups. It is a colorless solid that is soluble in organic solvents, but poorly soluble in water. It has been in commercial use since 1957.

BPA is a starting material for the synthesis of plastics, primarily

...

Read more

Intrinsic Properties

Structural Identifiers

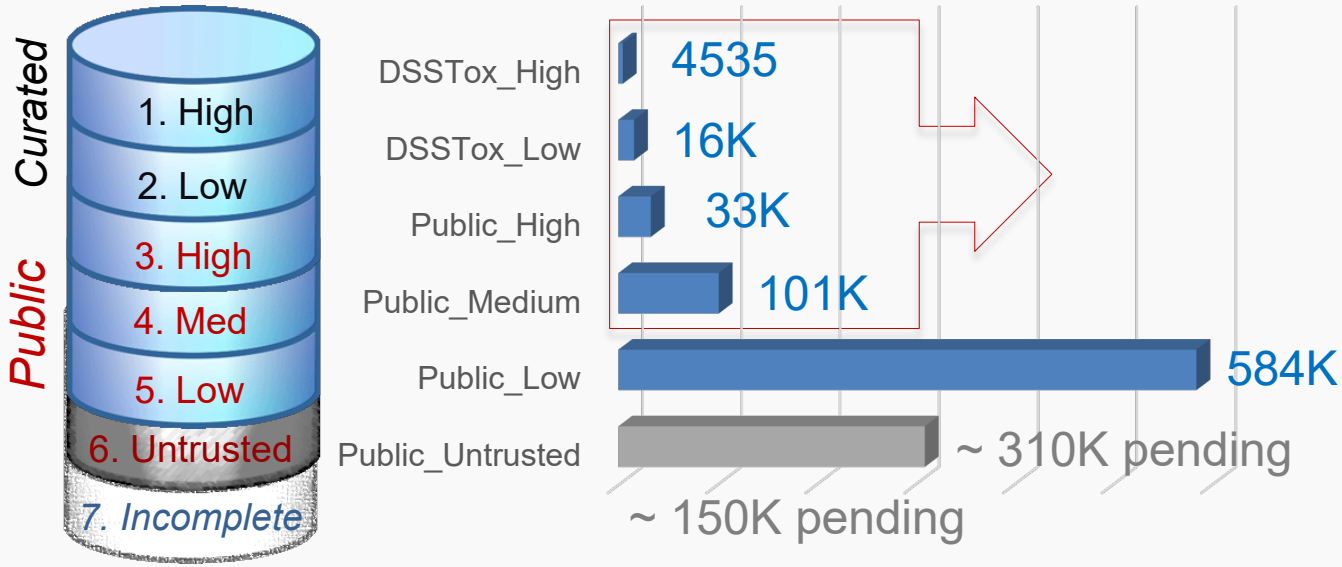
Linked Substances

Presence in Lists

Record Information

Quality Control Notes

Approximately 15 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

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

- And more…

Developing “NCCT Models”

- When we don’t have experimental data we predict the properties
- 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**

United States Environmental Protection Agency

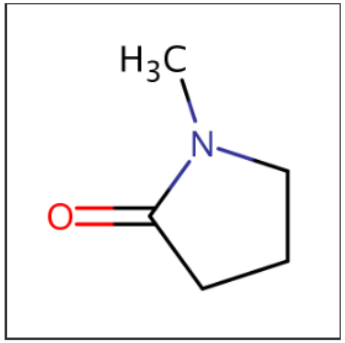
Home | Advanced Search | Batch Search | Lists | Predictions | Downloads | Share | Search all data

OPERA Models: LogP: Octanol-Water

Save PDF

N-Methyl-2-pyrrolidone

872-50-4 | DTXSID6020856



Model Results

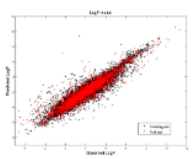
Predicted value: -0.300

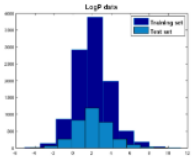
Global applicability domain: Inside

Local applicability domain index: 0.88

Confidence level: 0.81

Model Performance



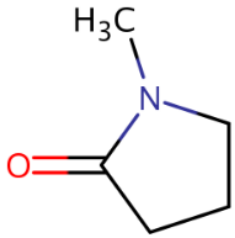


Weighted KNN model

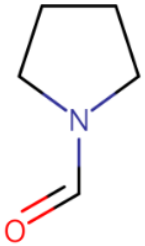
QMRF

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

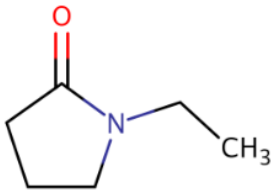
Nearest Neighbors from the Training Set



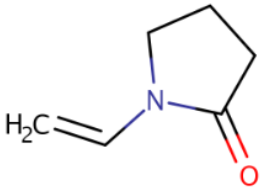
N-Methyl-2-pyrrolidone
Measured: -0.380
Predicted: -0.300



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

Access to Chemical Hazard Data

EPA United States Environmental Protection Agency

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Home | Advanced Search | Batch Search | Lists | Predictions | Downloads

Copy | Share | Submit Comment | Search all data

- DETAILS
- EXECUTIVE SUMMARY
- PROPERTIES
- ENV. FATE/TRANSPORT
- **HAZARD**
- ADME
- EXPOSURE
- BIOACTIVITY
- SIMILAR COMPOUNDS
- GENRA (BETA)
- RELATED SUBSTANCES
- SYNONYMS
- LITERATURE
- LINKS
- COMMENTS

Data Type

Point of Departure

Download

Human | Eco

Columns | 10 | Search query

More	Priority	Toxval type	Subtype	Risk assessment class	Value	Units	Study type	Exposure route	Species	Subsource	Source
	5	BMDL-10	-	chronic	0.609	mg/kg-day	human	-	mouse	EFSA CEF	EFSA
	5	NOEL	Systemic	repeat dose	3.75	mg/kg-day	repeat dose toxicity : oral	oral	rat	-	ECHA
	6	NOAEL	-	reproductive	3.75	mg/kg-day	reproductive	oral	rat	-	HPVIS
	5	NOEL	Systemic	repeat dose	3.75	mg/kg-day	repeat dose toxicity : oral	oral	rat	-	ECHA
	5	NOEL	Systemic	repeat dose	4.5	mg/kg-day	repeat dose toxicity : oral	oral	mouse	-	ECHA
	5	NOEL	Systemic	repeat dose	4.5	mg/kg-day	repeat dose toxicity : oral	oral	mouse	-	ECHA
	7	LEL	-	subchronic	5	mg/kg-day	subchronic	oral	rat	unpublished_submission	ToxRefDB
	7	nel	-	chronic	5	mg/kg-day	reproductive multigeneration	oral	rat	open_lit	ToxRefDB
	5	NOAEL	-	chronic	5	mg/kg-day	human	-	mouse	EFSA AFC	EFSA
	7	nel	-	subchronic	5	mg/kg-day	subchronic	oral	rat	unpublished_submission	ToxRefDB

Hazard Data from “ToxVal_DB”

- ToxVal Database contains following data:
  - 30,050 chemicals
  - 772,721 toxicity values
  - 29 sources of data
  - 21,507 sub-sources
  - 4585 journals cited
  - 69,833 literature citations

Sources of Exposure to Chemicals

EPA United States Environmental Protection Agency

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

Bisphenol A

80-05-7 | DTXSID7020182

Searched by DSSTox Substance Id.

- DETAILS
- EXECUTIVE SUMMARY
- PROPERTIES
- ENV. FATE/TRANSPORT
- HAZARD
- ADME
- **EXPOSURE**
  - **PRODUCT & USE CATEGORIES**
  - CHEMICAL WEIGHT FRACTION
  - CHEMICAL FUNCTIONAL USE
  - TOXICS RELEASE INVENTORY
  - MONITORING DATA
  - EXPOSURE PREDICTIONS
  - PRODUCTION VOLUME

Product and Use Categories (PUCs)

Download | Columns | 10 | Search query

Product or Use Categorization	Categorization type	Number of Unique Products
manufacturing, metals	CPCat Cassette	17
adhesive	CPCat Cassette	17
	CPCat Cassette	16
	CPCat Cassette	12
	CPCat Cassette	11
	CPCat Cassette	8
	CPCat Cassette	8
	CPCat Cassette	8
	CPCat Cassette	7
	CPCat Cassette	6

First | << | < | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | > | >> | Last

What chemicals in what product and use categories?

EPA United States Environmental Protection Agency

Methylparaben

99-76-3 | DTXSID4022529

Searched by Synonym from Valid Source.

Download

Columns 10

Product or Use Categorization
personal care: eye liner
personal care: body wash
personal care: sunscreen
personal care: hair conditioning treatment
personal care: lip color

What chemicals in what product and use categories?

EPA United States Environmental Protection Agency

Searched by Product & Use Categories

Results for CPDat Product Category: Personal Care: Eye Liner

182 chemicals

Download / Send

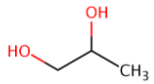
Sort by: DTXSID

Show info: DTXSID × CASRN × TOXCAST ×

Select all

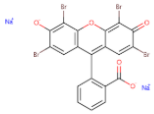
Filter by: Name or CASRN

Hide



1,2-Propylene glycol
DTXSID: DTXSID0021206
CASRN: 57-55-6
TOXCAST: 11/539

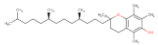
cis-Oleyl alcohol
DTXSID: DTXSID0022010
CASRN: 143-28-2
TOXCAST: 0



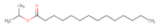
Eosin
DTXSID: DTXSID0025234
CASRN: 17372-87-1
TOXCAST: 45/302

1 related chemical structure with this substance

Polyvinylpyrrolidone
DTXSID: DTXSID0025941
CASRN: 9003-39-8
TOXCAST: 0



alpha-Vitamin E
DTXSID: DTXSID0026339
CASRN: 59-02-9
TOXCAST: 0



Isopropyl tetradecanoate
DTXSID: DTXSID0026838
CASRN: 110-27-0
TOXCAST: 1/299

0 related chemical structures with this substance

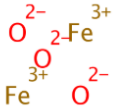
Paraffin waxes and Hydrocarbon waxes...
DTXSID: DTXSID0028115
CASRN: 63231-60-7
TOXCAST: 0

1 related chemical structure with this substance

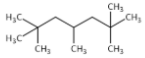
Alcohols, C16-18
DTXSID: DTXSID0028323
CASRN: 67762-27-0
TOXCAST: 1/163

0 related chemical structures with this substance

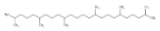
Fats and Glyceridic oils, vegetable, hyd...
DTXSID: DTXSID0028454
CASRN: 68334-28-1
TOXCAST: 0



Iron(III) oxide
DTXSID: DTXSID0029632
CASRN: 1309-37-1
TOXCAST: 0



2,2,4,6,6-Pentamethylheptane
DTXSID: DTXSID0042034
CASRN: 13475-82-6
TOXCAST: 0



Squalane
DTXSID: DTXSID0046513
CASRN: 111-01-3
TOXCAST: 2/109

Remember home page searches
Searching for “eye”…

Chemicals | Product/Use Categories | Assay/Gene

eye

Eyeness
DTXSID7041099

Eyesule

Chemicals | Product/Use Categories | Assay/Gene

eye

CPDat PRODUCT category: personal care eye cream
creams and moisturizers for specific treatment of eye area

CPDat PRODUCT category: personal care eye drops
products for lubricating eyes or treating redness

CPDat PRODUCT category: personal care eye liner
eye liners or brow coloring products (liquid or gel formulation specified)

Chemicals | Product/Use Categories | Assay/Gene

eye

ASSAY: Tanguay_ZF_120hpf_EYE_up

In Vitro Bioassay Screening

ToxCast and Tox21

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

Bisphenol A

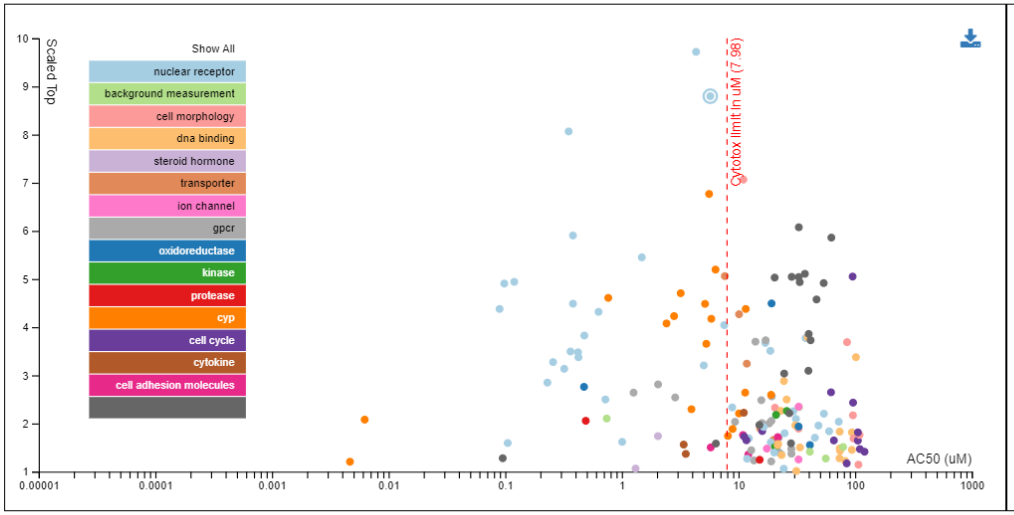
80-05-7 | DTXSID7020182

Searched by DSSTox Substance Id.

- DETAILS
- EXECUTIVE SUMMARY
- PROPERTIES
- ENV. FATE/TRANSPORT
- HAZARD
- ADME
- EXPOSURE
- BIOACTIVITY
  - TOXCAST: SUMMARY
  - PUBCHEM
  - TOXCAST: DATA
  - TOXCAST: MODELS
- SIMILAR COMPOUNDS
- GENRA (BETA)
- RELATED SUBSTANCES

Chemical Activity Summary

TOXCAST DATA



ASSAY DETAILS

AC50 (uM): 5.73
Scaled top: 8.80
Assay Endpoint Name: OT_ER_ERaERa_0480
Assay Description: 742
Gene Symbol: ESR1
Organism: human
Tissue: kidney
Assay Format Type: cell-based
Biological Process Target: protein stabilization
Detection Technology: Protein-fragment Complementation
Analysis Direction: positive
Intended Target Family: nuclear receptor
Description: Data from the assay component OT_ER_ERaERa_0480 was analyzed into 1 assay endpoint. This assay endpoint, OT_ER_ERaERa_0480, was analyzed in the positive fitting direction relative to DMSO as the negative control and baseline of activity. Using a type of binding reporter, measures of receptor for gain-of-signal activity can be used to understand the binding at the pathway-level as they relate to the gene ESR1. Furthermore, this assay endpoint can be referred to as a primary readout, because the performed assay has only produced 1 assay endpoint. To generalize the intended target to other relatable targets, this assay endpoint is annotated to the 'nuclear receptor' intended target family, where the subfamily is 'steroidal'.

In Vitro Bioassay Screening

ToxCast and Tox21

Download

Columns 10

- Name
- Modal
- Description
- SeqaPASS
- Gene Name
- AOP
- Event
- Hit Call
- Top
- Scaled Top
- AC50
- logAC50
- Intended Target Family

Search query | Show Inactive | Show Background

Description	SeqaPASS	Gene Name	AOP	Event	Hit Call	Top	Scaled Top	AC50	logAC50	Intended Target Family
-	-	-	-	-	ACTIVE	35.5	1.65	65.8	1.82	cell cycle
2	NP_000116.2	ESR1	200	1181	ACTIVE	109	4.49	0.381	-0.419	nuclear receptor
-	-	-	-	-	ACTIVE	1.20	1.81	106	2.02	cell cycle
-	-	-	-	-	ACTIVE	0.874	1.76	109	2.04	cell morphology
-	-	-	-	-	ACTIVE	5.92	7.07	11.0	1.04	cell morphology
-	-	-	-	-	ACTIVE	1.20	1.47	110	2.04	cell cycle
-	-	-	-	-	ACTIVE	4.49	5.05	95.2	1.98	cell cycle
-	-	-	-	-	ACTIVE	2.71	3.69	85.3	1.93	cell morphology
-	-	-	-	-	ACTIVE	1.66	1.17	84.7	1.93	cell cycle
-	-	-	-	-	ACTIVE	1.80	1.65	106	2.02	cell cycle

First << < 1 2 3 4 5 6 7 8 9 10 > >> Last

Showing 1 to 10 of 161 records

In Vitro Bioassay Screening

ToxCast and Tox21

Download

Columns 10

Search query | Show Inactive | Show Background

Name	Modal	Description	SeqaPASS	Gene Name	AOP	Event	Hit Call	Top	Scaled Top	AC50	logAC50	Intended Target Family
ACEA_T47D_80hr_Negative		-	-	-	-	-	ACTIVE	35.5	1.65	65.8	1.82	cell cycle
ACEA_T47D_80hr_Positive		-	NP_000116.2	ESR1	200	1181	ACTIVE	109	4.49	0.381	-0.419	nuclear receptor
APR_HepG2_CellLoss_24h_dn		-	-	-	-	-	ACTIVE	1.20	1.81	106	2.02	cell cycle
APR_HepG2_MitoMass_24h_dn		-	-	-	-	-	ACTIVE	0.874	1.76	109	2.04	cell morphology
APR_HepG2_MitoMembPot_24h_dn		-	-	-	-	-	ACTIVE	5.92	7.07	11.0	1.04	cell morphology
APR_HepG2_OxidativeStress_24h_up		-	-	-	-	-	ACTIVE	1.20	1.47	110	2.04	cell cycle
APR_HepG2_CellLoss_72h_dn		-	-	-	-	-	ACTIVE	4.49	5.05	95.2	1.98	cell cycle
APR_HepG2_MitoMembPot_72h_dn		-	-	-	-	-	ACTIVE	2.71	3.69	85.3	1.93	cell morphology
APR_HepG2_MitoticArrest_72h_up		-	-	-	-	-	ACTIVE	1.66	1.17	84.7	1.93	cell cycle
APR_HepG2_OxidativeStress_72h_up		-	-	-	-	-	ACTIVE	1.80	1.65	106	2.02	cell cycle

First << < 1 2 3 4 5 6 7 8 9 10 > >> Last

Showing 1 to 10 of 161 records

Assay Modal Details

All Chemicals in Assay Endpoint: ACEA_T47D_80hr_Negative

Annotations | Citations | tcpl Processing | Reagents | AOPs

Excel

Aeid	1
Entrez Gene Id	0
Gene Name	
Gene Symb	
Assay Sour	
Assay Sour	
Assay Name	
Assay Desc	
Timepoint H	
Organism	
Tissue	
Cell Format	
Cell Free Component Source	
Cell Short Name	
Cell Growth Mode	
Assay Footprint	

All Chemicals in Assay Endpoint: ACEA_T47D_80hr_Negative

Annotations | Citations | tcpl Processing | Reagents | AOPs

Excel

	PMID	url	Title	Author	Citation	doi
1	16481145	PubMed URL	Microelectronic cell sensor assay for detection of cytotoxicity and prediction of acute toxicity	Xing JZ, Zhu L, Gabos S, Xie L	Xing JZ, Zhu L, Gabos S, Xie L. Microelectronic cell sensor assay for detection of cytotoxicity and prediction of acute toxicity. Toxicol In Vitro. 2006 Sep;20(6):995-1004. Epub 2006 Feb 14. PubMed PMID: 16481145.	
2	23682706					

All Chemicals in Assay Endpoint: ACEA_T47D_80hr_Negative

Annotations | Citations | tcpl Processing | Reagents | AOPs

Excel

	Assay Run Type	Level Applied	Method Name	Description
1	MULTI	level2	none	apply no level 2 method
2	MULTI	level3	bval.apid.nwllslowconc.med	Take the median cval of the n wells and the first two concentrations, by apid
3	MULTI	level3	pval.apid.mednc byconc.min	plate-wise meidan based on negative control, (min)
4	MULTI			
5	MULTI			
6	MULTI			
7	MULTI			
8	MULTI			

All Chemicals in Assay Endpoint: ACEA_T47D_80hr_Negative

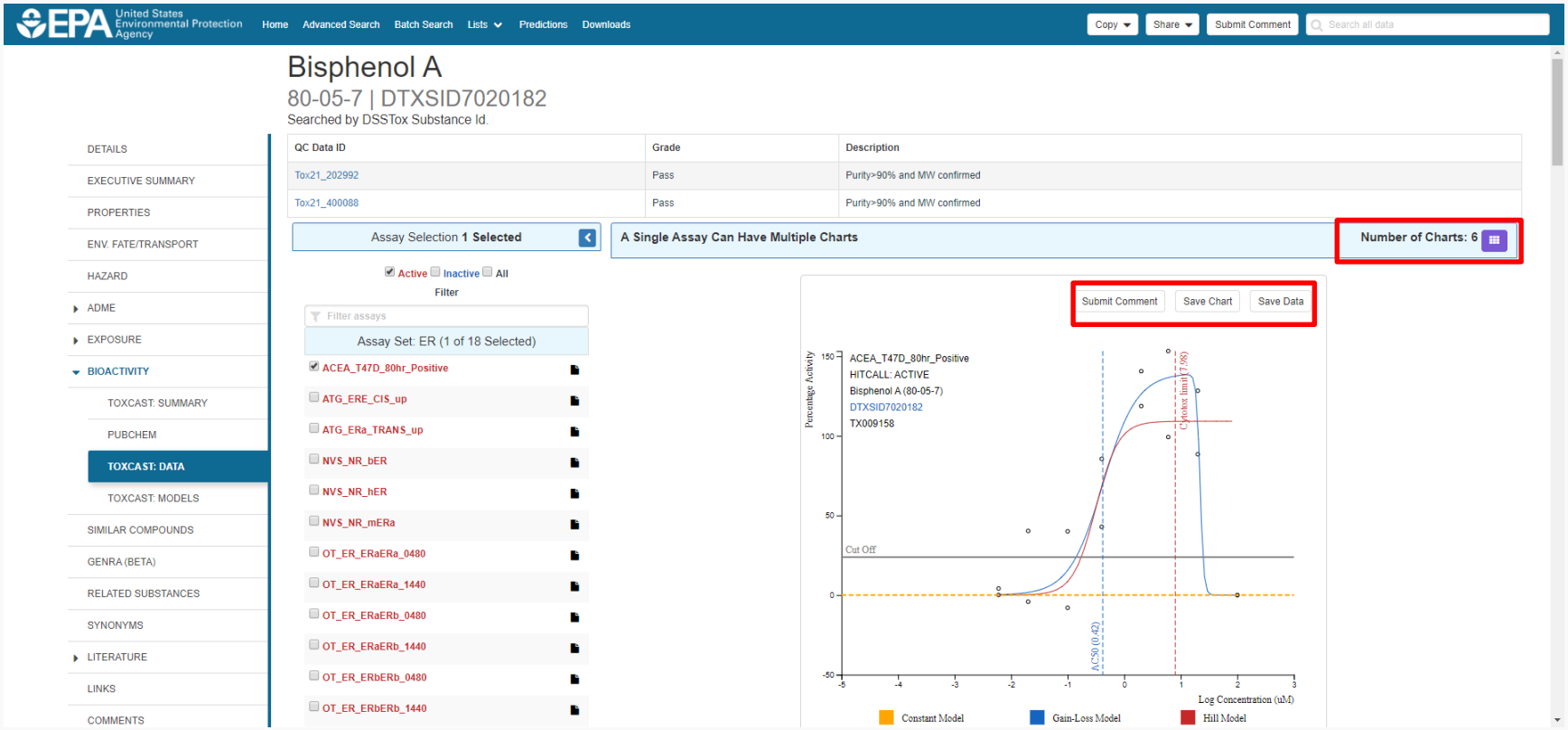
Annotations | Citations | tcpl Processing | Reagents | AOPs

Excel

	Reagent Type	Reagent Value	Culture or Assay
1	media_base	RPMI-1640	culture
2	media_serum	10% FBS	culture
3	media_temp_celcius	37	culture
4	media_time_hr_min	24	culture
5	media_cell_aliquot	20000	culture
6	media_base	RPMI-1640	assay
7	media_serum	10% charcoal-stripped FBS	assay
8	media_temp_celcius_min	37	assay
9	media_time_hr	80	assay

In Vitro Bioassay Screening

ToxCast and Tox21



In Vitro Bioassay Screening

Multi-chart Display

EPA United States Environmental Protection Agency

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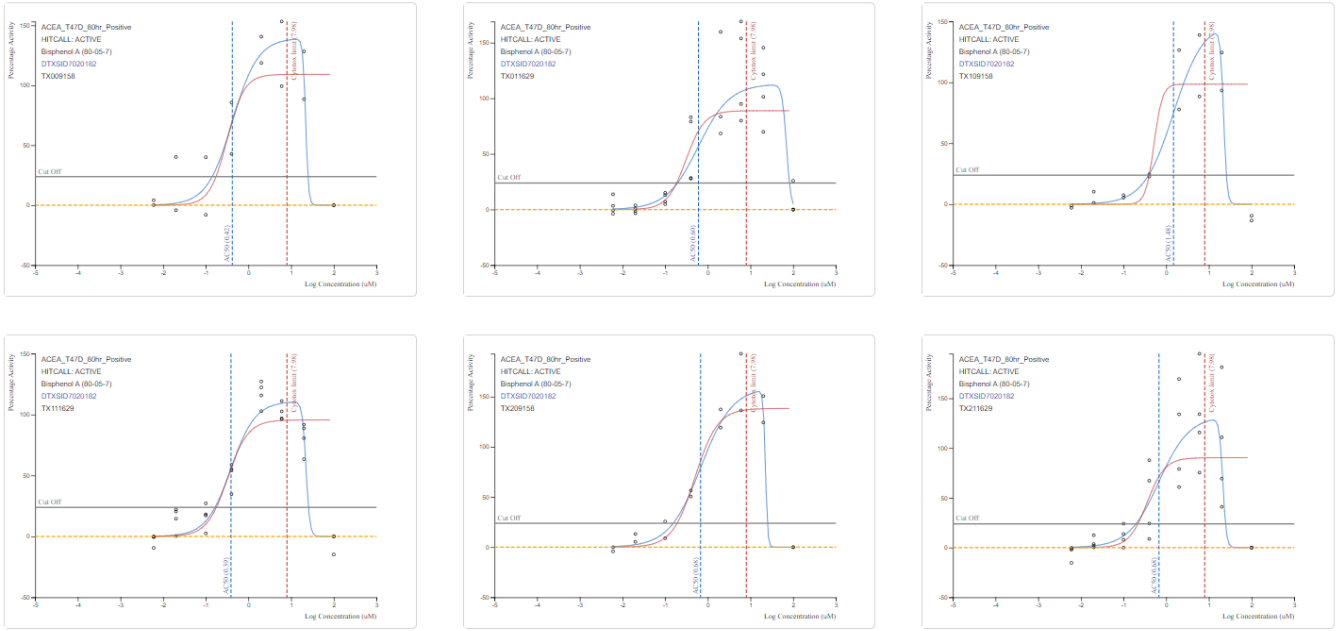
- PROPERTIES
- ENV. FATE/TRANSPORT
- HAZARD
- ADME
- EXPOSURE
- BIOACTIVITY
  - TOXCAST: SUMMARY
  - PUBCHEM
  - TOXCAST: DATA
  - TOXCAST: MODELS
- SIMILAR COMPOUNDS
- GENRA (BETA)
- RELATED SUBSTANCES
- SYNONYMS
- LITERATURE
- LINKS
- COMMENTS

Tox21_400088	Pass	Purity>90% and MW confirmed

A Single Assay Can Have Multiple Charts — Number of Charts: 6



Assay Modal Details

All Chemicals in Assay Endpoint: ACEA_T47D_80hr_Negative

Annotations | Citations | tcpl Processing | Reagents | AOPs

Excel

Aeid	1
Entrez Gene Id	0
Gene Name	
Gene Symb	
Assay Sour	
Assay Sour	
Assay Name	
Assay Desc	
Timepoint H	
Organism	
Tissue	
Cell Format	
Cell Free Component Source	
Cell Short Name	
Cell Growth Mode	
Assay Footprint	

All Chemicals in Assay Endpoint: ACEA_T47D_80hr_Negative

Annotations | Citations | tcpl Processing | Reagents | AOPs

Excel

	PMID	url	Title	Author	Citation	doi
1	16481145	PubMed URL	Microelectronic cell sensor assay for detection of cytotoxicity and prediction of acute toxicity	Xing JZ, Zhu L, Gabos S, Xie L	Xing JZ, Zhu L, Gabos S, Xie L. Microelectronic cell sensor assay for detection of cytotoxicity and prediction of acute toxicity. Toxicol In Vitro. 2006 Sep;20(6):995-1004. Epub 2006 Feb 14. PubMed PMID: 16481145.	
2	23682706					

All Chemicals in Assay Endpoint: ACEA_T47D_80hr_Negative

Annotations | Citations | tcpl Processing | Reagents | AOPs

Excel

	Assay Run Type	Level Applied	Method Name	Description
1	MULTI	level2	none	apply no level 2 method
2	MULTI	level3	bval.apid.nwllslowconc.med	Take the median cval of the n wells and the first two concentrations, by apid
3	MULTI	level3	pval.apid.mednctbyconc.min	plate-wise meidan based on negative control, (min)
4	MULTI			
5	MULTI			
6	MULTI			
7	MULTI			
8	MULTI			

All Chemicals in Assay Endpoint: ACEA_T47D_80hr_Negative

Annotations | Citations | tcpl Processing | Reagents | AOPs

Excel

	Reagent Type	Reagent Value	Culture or Assay
1	media_base	RPMI-1640	culture
2	media_serum	10% FBS	culture
3	media_temp_celcius	37	culture
4	media_time_hr_min	24	culture
5	media_cell_aliquot	20000	culture
6	media_base	RPMI-1640	assay
7	media_serum	10% charcoal-stripped FBS	assay
8	media_temp_celcius_min	37	assay
9	media_time_hr	80	assay

List of Chemicals for an Assay

Assay Endpoint Name: ACEA_T47D_80hr_Negative

Assay Details

Assay Endpoint Name: ACEA_T47D_80hr_Negative

Assay Source Description: ACEA Biosciences, Inc. (ACEA) is a privately owned biotechnology company that developed a real-time, label-free, cell-based assay system based on a microelectronic readout called xCELLigence.

1813 chemicals

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Show info: DTXSID × CASRN × TOXCAST ×

Select all

Sort by: DTXSID

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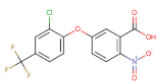
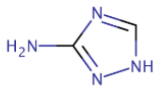
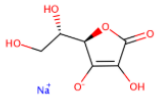
Hide



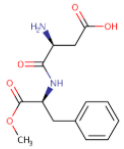
Acifluorfen
DTXSID: DTXSID0020022
CASRN: 50594-66-6
TOXCAST: 23/694



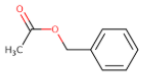
Amitrole
DTXSID: DTXSID0020076
CASRN: 61-82-5
TOXCAST: 1/303



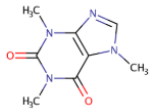
Sodium L-ascorbate
DTXSID: DTXSID0020105
CASRN: 134-03-2
TOXCAST: 19/561



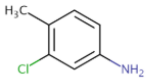
Aspartame
DTXSID: DTXSID0020107
CASRN: 22839-47-0
TOXCAST: 1/296

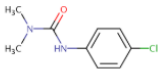


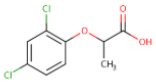
Benzyl acetate
DTXSID: DTXSID0020151
CASRN: 140-11-4
TOXCAST: 1/298

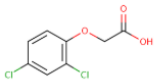


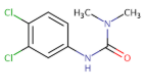
Caffeine
DTXSID: DTXSID0020232
CASRN: 58-08-2
TOXCAST: 21/546



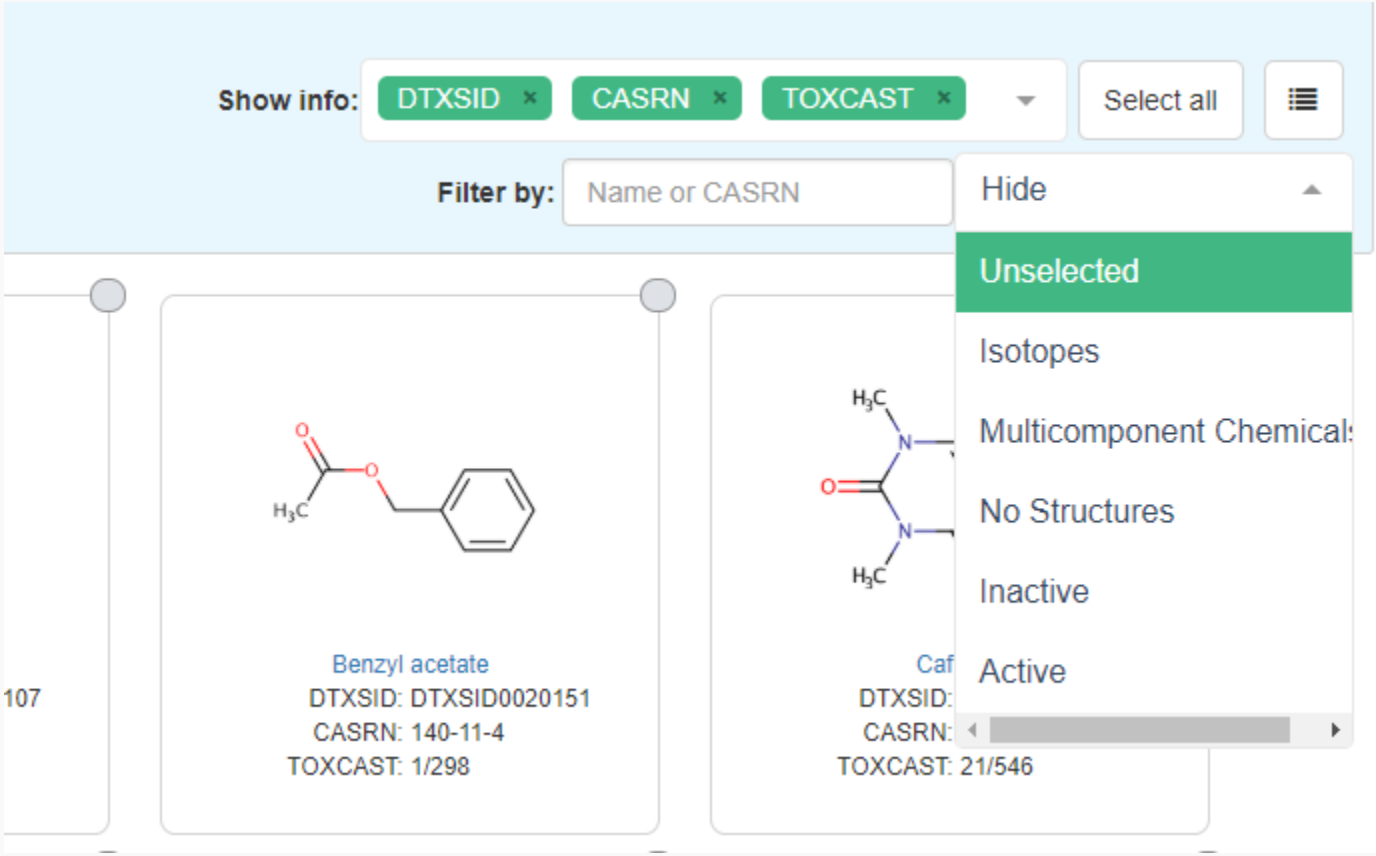






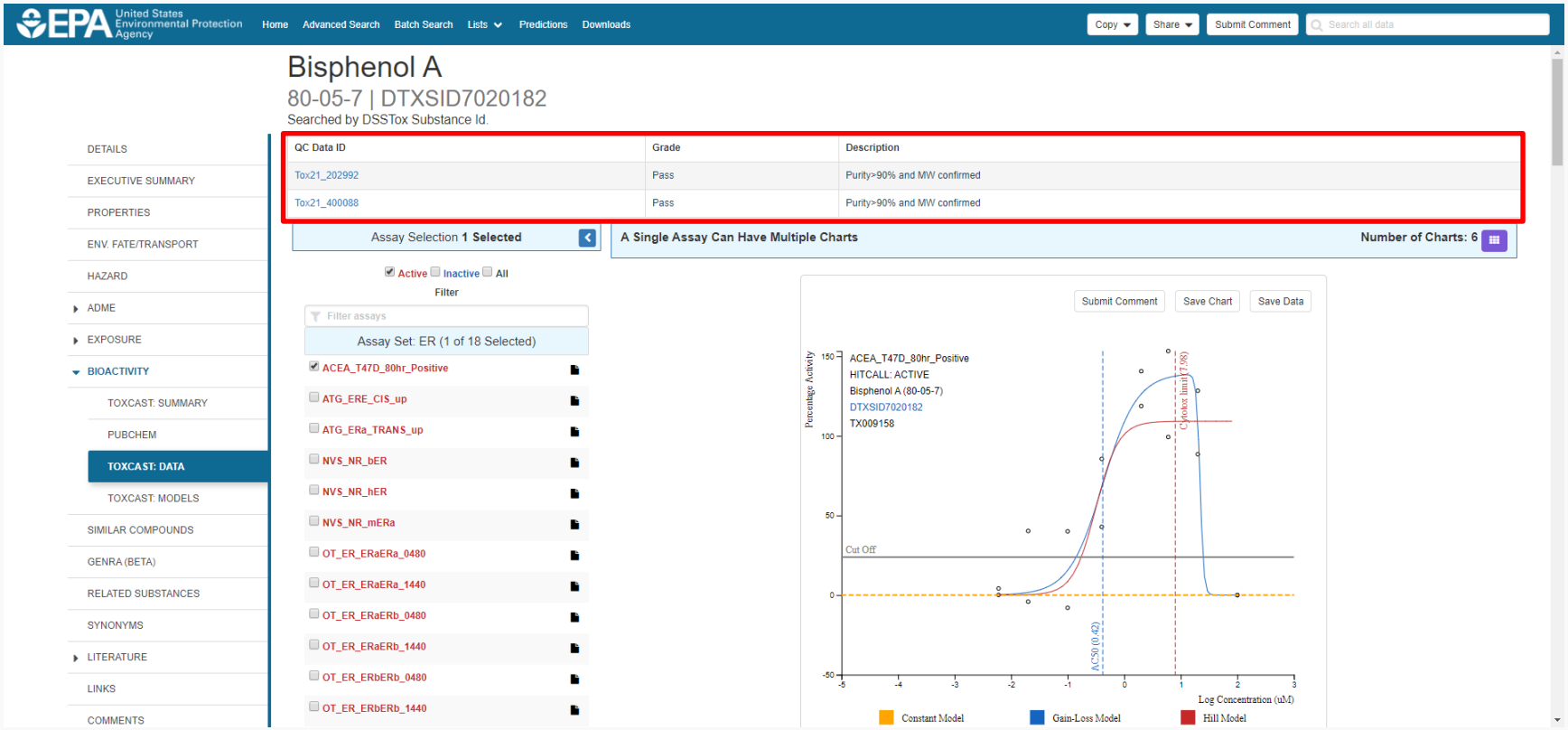


Choose Display Details



In Vitro Bioassay Screening

ToxCast and Tox21



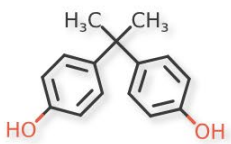
Access to Analytical QC Data

Tox21

Structure Search | Search...

Home / Tox21 Samples / Tox21_202992

Bisphenol A



QC Grade

T0	A	MW Confirmed, Purity > 90%
T4	A	MW Confirmed, Purity > 90%

Identifiers

Tox21	Tox21_202992
NCATS	NCGC00260537-01
CAS	80-05-7
PubChem	144210190

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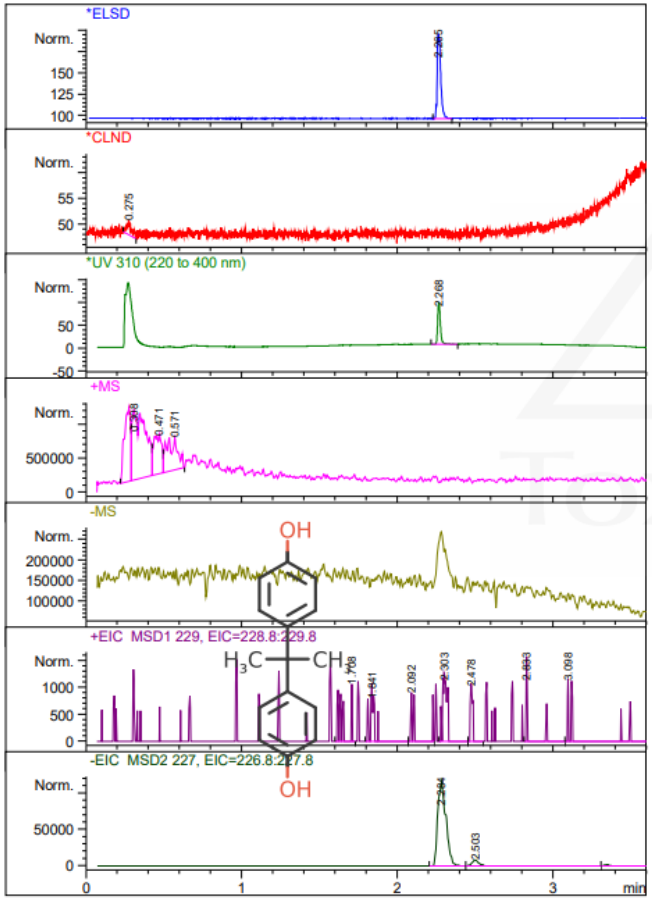
National Center for Advancing Translational Sciences (NCATS), 6701 Democracy Boulevard, Bethesda MD 20892-4874 • 301-435-0888

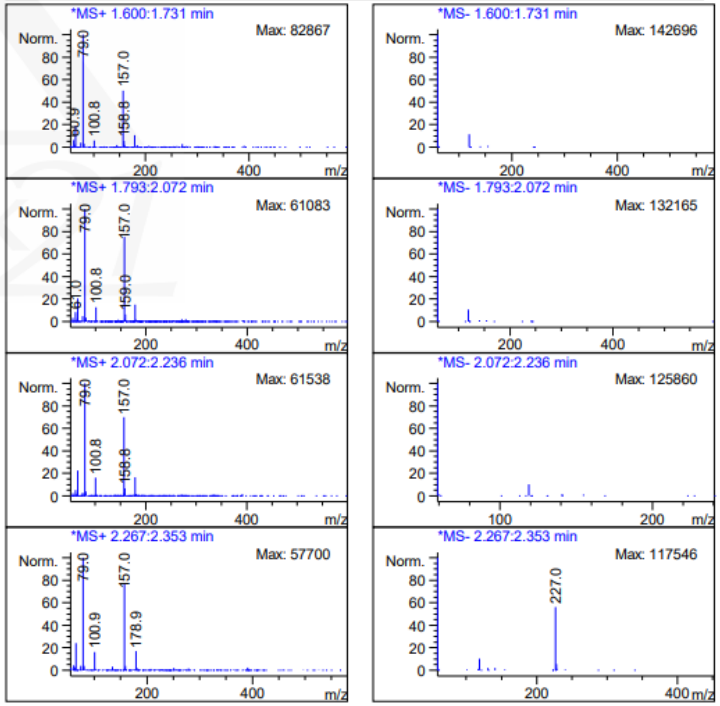
Access to Analytical QC Data

ID Tox21_202992 Plate Batch3-SP115973 Well P1-D-09 File SP115973_D009.D Inj Date: 5 May 12 1:33 am - MF C15H16O2 MW 228.1 Expected Conc: 2.97 mM



RT	Found	ELS%	UV %	ELS[mg/mL]	Adj[ELS]	[N mM]	Adj[CLN]	#N
1.71		0.0	0.0					0.0
1.84		0.0	0.0					0.0
2.09		0.0	0.0					0.0
2.27	Yes	100.0	100.0	1.76	7.73 mM			0.0

Comment: Passed



PubChem

MW Confirmed, Purity>90%

OpAns_Process.MAC Version A.01.10 - Dec 9, 2010

Page 1 of 1

Related Substances
e.g. Transformation Products

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Chlorothalonil

1897-45-6 | DTXSID0020319

Searched by DSSTox Substance Id.

- DETAILS
- EXECUTIVE SUMMARY
- PROPERTIES
- ENV. FATE/TRANSPORT
- HAZARD
- ADME
- EXPOSURE
- BIOACTIVITY
- SIMILAR COMPOUNDS
- GENRA (BETA)
- **RELATED SUBSTANCES**
- SYNONYMS
- LITERATURE
- LINKS
- COMMENTS

8 chemicals

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Sort by: Relationship | Filter by: Name or CASRN | Hide

Searched Chemical
Chlorothalonil
DTXSID: DTXSID0020319
CASRN: 1897-45-6

Transformation Product
4-Hydroxy-2,5,6-trichloroisophthalonitrile
DTXSID: DTXSID90182586
CASRN: 28343-61-5

Transformation Product
3-Carbamoyl-2,4,5-trichlorobenzoic acid
DTXSID: DTXSID10597537
CASRN: 142733-37-7

Transformation Product
2,4-dicarbamoyl-3,5,6-trichlorobenzene...
DTXSID: DTXSID30891327
CASRN: NOCAS_891327

Transformation Product
3-carbamoyl-2,5,6-trichloro-4-hydroxyb...
DTXSID: DTXSID90891328
CASRN: NOCAS_891328

Transformation Product
4-carbamoyl-2,5-dichloro-6-cyanobenz...
DTXSID: DTXSID50891329
CASRN: NOCAS_891329

Transformation Product
2-carbamoyl-3,5,6-trichloro-4-cyanoben...
DTXSID: DTXSID60891330
CASRN: NOCAS_891330

Transformation Product
2,5-dichloro-4,6-dicyanobenzene-1,3-di...
DTXSID: DTXSID20891331
CASRN: NOCAS_891331

UVCB Chemicals

EPA United States Environmental Protection Agency

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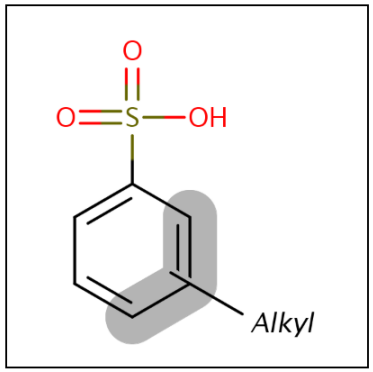
(C10-C16) Alkylbenzenesulfonic acid

68584-22-5 | DTXSID2028723

Searched by CAS-RN.

- DETAILS
- RELATED SUBSTANCES
- PROPERTIES
- ENV. FATE/TRANSPORT
- BIOACTIVITY
- SYNONYMS
- COMMENTS



Intrinsic Properties

Molecular Formula: Not Found | Mol File | Find All Chemicals

Average Mass: 0 g/mol | Isotope Mass Distribution

Monoisotopic Mass: 0 g/mol

Presence in Lists

Federal

- Endocrine Disruptor Screening Program (EDSP) Universe of Chemicals
- EPAHFR Table H-2 - Chemicals in hydraulic fracturing fluids from 2005-2013
- TSCA Inventory, active non-confidential portion
- ECOTOXicology knowledgebase (ECOTOX)
- TOX21SL: Tox21 Screening Library
- EPAHFR - EPA Chemicals associated with hydraulic fracturing

US State

None.

International

None.

Other

- SUSDAT: The NORMAN Network Suspect Screening List
- TSCA Workplan Step 2 Chemicals
- Surfactant List Screened in Swiss Wastewater (2014)

Related Substances for UVCB Chemicals

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DETAILS
RELATED SUBSTANCES
PROPERTIES
ENV. FATE/TRANSPORT
BIOACTIVITY
SYNONYMS
COMMENTS

27 chemicals

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Show info: DTXSID × CASRN × TOXCAST × Select all

Sort by: Relationship

Filter by: Name or CASRN Hide

Searched Chemical
(C10-C16) Alkylbenzenesulfonic acid
DTXSID: DTXSID2028723
CASRN: 68584-22-5
TOXCAST: 15/113

Predecessor: Component
Alkylbenzenesulfonate, linear
DTXSID: DTXSID3020041
CASRN: 42615-29-2
TOXCAST: 0

Component
C10-linear alkylbenzenesulfonate
DTXSID: DTXSID70891689
CASRN: NOCAS_891689
TOXCAST: 0

Component
C12-linear alkyl benzene sulfonate
DTXSID: DTXSID90891641
CASRN: NOCAS_891641
TOXCAST: 0

Component
4-(decan-4-yl)benzenesulfonic acid
DTXSID: DTXSID40891333
CASRN: NOCAS_891333
TOXCAST: 0

Component
4-(decan-5-yl)benzene-1-sulfonic acid
DTXSID: DTXSID70881146
CASRN: NOCAS_881146
TOXCAST: 0

Component
4-(undecan-5-yl)benzene-1-sulfonic acid
DTXSID: DTXSID40881097
CASRN: NOCAS_881097
TOXCAST: 0

Component
4-Tetradecylbenzenesulfonic acid
DTXSID: DTXSID1068489
CASRN: 47377-16-2
TOXCAST: 0

Component
4-(dodecan-4-yl)benzene-1-sulfonic acid
DTXSID: DTXSID30862870
CASRN: NOCAS_862870
TOXCAST: 0

Component
4-(Dodecan-6-yl)benzene-1-sulfonic acid
DTXSID: DTXSID30860093
CASRN: 23003-92-1
TOXCAST: 0

Markush Child

Markush Child

Markush Child

Markush Child

Markush Child

Identifiers to Support Searches

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Bisphenol A

80-05-7 | DTXSID7020182

Searched by DSSTox Substance Id.

- DETAILS
- EXECUTIVE SUMMARY
- PROPERTIES
- ENV. FATE/TRANSPORT
- HAZARD
- ADME
- EXPOSURE
- BIOACTIVITY
- SIMILAR COMPOUNDS
- GENRA (BETA)
- RELATED SUBSTANCES
- **SYNONYMS**
- LITERATURE
- LINKS
- COMMENTS

25 | Search query

Synonym	Quality
Bisphenol A	**Valid**
4,4'-(Propane-2,2-diyl)diphenol	**Valid**
Phenol, 4,4'-(1-methylethylidene)bis-	**Valid**
80-05-7 Active CAS-RN	**Valid**
BPA	**Valid**
4,4'-Propane-2,2-diyldiphenol	**Valid**
Phenol, 4,4'-(1-methylethylidene)bis-	**Valid**
4-06-00-06717 Beilstein Registry Number	Beilstein
(4,4'-Dihydroxydiphenyl)dimethylmethane	*Good*
2,2-Bis(4'-hydroxyphenyl) propane	*Good*
2,2'-Bis(4-hydroxyphenyl)propane	*Good*
2,2-BIS-(4-HYDROXY-PHENYL)-PROPANE	*Good*
2,2-Bis(4-hydroxyphenyl)propane	*Good*
2,2-Bis(p-hydroxyphenyl)propane	*Good*
2,2-Di(4-Hydroxyphenyl) Propane	*Good*

Literature Searches and Links

EPA United States Environmental Protection Agency

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Bisphenol A

80-05-7 | DTXSID7020182

Searched by DSSTox Substance Id.

- DETAILS
- EXECUTIVE SUMMARY
- PROPERTIES
- ENV. FATE/TRANSPORT
- LITERATURE
  - GOOGLE SCHOLAR
  - **PUBMED ABSTRACT SIFTER**
  - PUBCHEM ARTICLES
  - PUBCHEM PATENTS
  - PPRTV
  - IRIS

1) Select PubMed starting point query then 2) click on Retrieve.

Select a Query Term | Retrieve Articles

- Select a 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

Optionally, edit the query before retrieving.

"80-05-7" OR "Bisphenol A"

Abstract Sifter – PubMed Integration searching >28 million abstracts

EPA United States Environmental Protection Agency

Bisphenol A

80-05-7 | DTXSID7020182

Searched by DSSTox Substance Id.

- DETAILS
- EXECUTIVE SUMMARY
- PROPERTIES
- ENV. FATE/TRANSPORT
- HAZARD
- ADME
- EXPOSURE
- BIOACTIVITY
- GENRA (BETA)
- SIMILAR COMPOUNDS
- RELATED SUBSTANCES
- SYNONYMS
- LITERATURE
  - GOOGLE SCHOLAR
  - PUBMED ABSTRACT SIFTER
  - PUBCHEM ARTICLES
  - PUBCHEM PATENTS

1) Select PubMed starting point query then 2) click on Retrieve.

Hazard [Retrieve Articles]

118 of 118 articles loaded...

Optionally, edit the query before retrieving.

("80-05-7" OR "Bisphenol A") AND (NOAEL or NOEL OR LOEL or Rfd OR "reference dose" OR "reference concentration" OR "adverse effect level"[tiab] OR "cancer slope factor"[tiab])

To find articles quickly, enter terms to sift abstracts.

Download / Send to... [Download Sifter for Excel]

PMID	Year	Title	Authors	Journal	Rev
29573712	2018	Urinary bisphenol analogues and triclosan in children from south China and implications f...	Chen; Fang; Ren; Fan; Zhang; Liu; Zhou; Chen; Yu;...	Environmental pollution (Barking, Essex : 1987)	
29306804	2018	Phosphorus flame retardants and Bisphenol A in indoor dust and PM2.5 in kindergartens ...	Deng; Li; Wu; Richard; Wang; Ho	Environmental pollution (Barking, Essex : 1987)	
29268159	2017	Presence of diphenyl phosphate and aryl-phosphate flame retardants in indoor dust from ...	Björnsdotter; Romera-García; Borrull; de Boer; Rubi...	Environment international	
29172986	2017	Bisphenol A and Bisphenol S release in milk under household conditions from baby bottle...	Russo; Barbato; Cardone; Fattore; Albrizio; Grumetto	Journal of environmental science and health. Part. ...	
29097150	2017	Prenatal bisphenol A (BPA) exposure alters the transcriptome of the neonate rat amygdal...	Arambula; Jima; Patisaul	Neurotoxicology	
28982642	2017	Systematic Review and Meta-Analysis of Early-Life Exposure to Bisphenol A and Obesity...	Wassenaar; Trasande; Legler	Environmental health perspectives	✓
28890130	2017	Effects of perinatal bisphenol A exposure on the volume of sexually-dimorphic nuclei of ju...	Arambula; Fuchs; Cao; Patisaul	Neurotoxicology	
28641706	2017	Delayed onset of puberty in male offspring from bisphenol A-treated dams is followed by t...	Oliveira; Romano; de Campos; Cavallin; Oliveira; R...	Reproduction, fertility, and development	
28608465	2017	Effect of bisphenol A on reproductive processes: A review of in vitro, in vivo and epidemiol...	Tomza-Marciniak; Stępkowska; Kuba; Pilarczyk	Journal of applied toxicology : JAT	✓
28503266	2017	Inhalation Toxicity of Bisphenol A and Its Effect on Estrous Cycle, Spatial Learning, and M...	Chung; Han; Lee; Lee	Toxicological research	
28377091	2017	Derivation of an oral Maximum Allowable Dose Level for Bisphenol A.	Goodman; Peterson; Hixon; Pacheco Shubin	Regulatory toxicology and pharmacology : RTP	✓
28257732	2017	Bisphenol A release from orthodontic adhesives measured in vitro and in vivo with gas ch...	Moreira; Matos; de Souza; Brigante; Queiroz; Roma...	American journal of orthodontics and dentofacial ort...	
28219029	2017	Versatile transduction scheme based on electrolyte-gated organic field-effect transistor us...	Piro; Wang; Benaoudia; Tibaldi; Anquetin; Noël; Rei...	Biosensors & bioelectronics	

External Links to ~80 websites
Growing list of out links -

EPA United States Environmental Protection Agency

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Bisphenol A

80-05-7 | DTXSID7020182

Searched by Approved Name.

- DETAILS
- EXECUTIVE SUMMARY
- PROPERTIES
- ENV. FATE/TRANSPORT
- HAZARD
- ADME
- EXPOSURE
- BIOACTIVITY
- SIMILAR COMPOUNDS
- GENRA (BETA)
- RELATED SUBSTANCES
- SYNONYMS
- LITERATURE
- **LINKS**
- COMMENTS

General

- EPA Substance Registry Service
- Household Products Database
- Chemical Entities of Biological Interest (ChEBI)
- PubChem
- Chemspider
- CPCat
- DrugBank
- HMDB
- Wikipedia
- MSDS Lookup
- ChEMBL
- Chemical Vendors
- CalEPA Office of Environmental Health Hazard Assessment
- NIOSH Chemical Safety Cards
- ToxPlanet
- ACS Reagent Chemicals
- Wikidata
- ChemHat: Hazards and Alternatives Toolbox
- Wolfram Alpha
- ScrubChem
- ECHA Brief Profile
- ECHA Infocard
- ChemAgora

Toxicology

- ACToR
- DrugPortal
- CCRIS
- ChemView
- CTD
- eChemPortal
- Gene-Tox
- HSDB

Publications

- Toxline
- Environmental Health Perspectives
- NIEHS
- National Toxicology Program
- Google Books
- Google Scholar
- Google Patents
- PPRTVWEB
- PubMed
- IRIS Assessments
- EPA HERO
- NIOSH Skin Notation Profiles
- NIOSH Pocket Guide
- RSC Publications
- BioCaddie DataMed
- Springer Materials
- Federal Register
- Regulations.gov
- Bielefeld Academic Search Engine
- CORE Literature Search

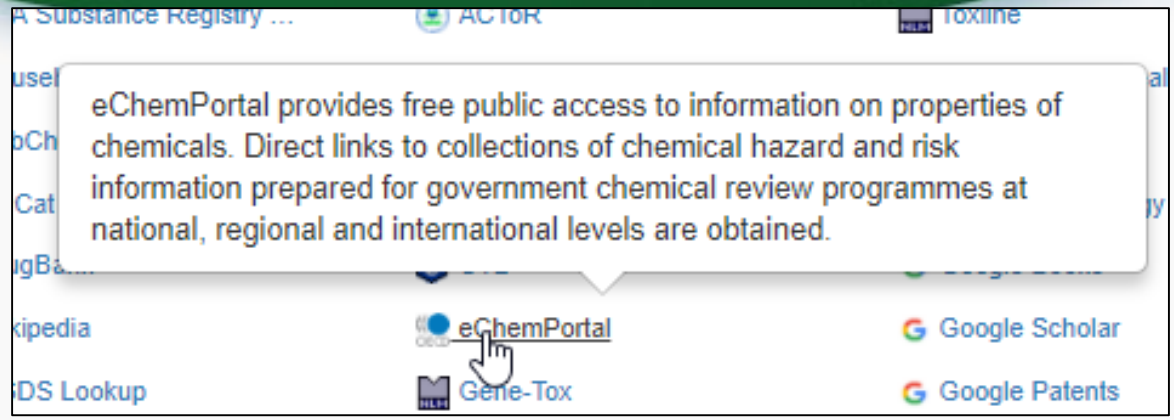
Analytical

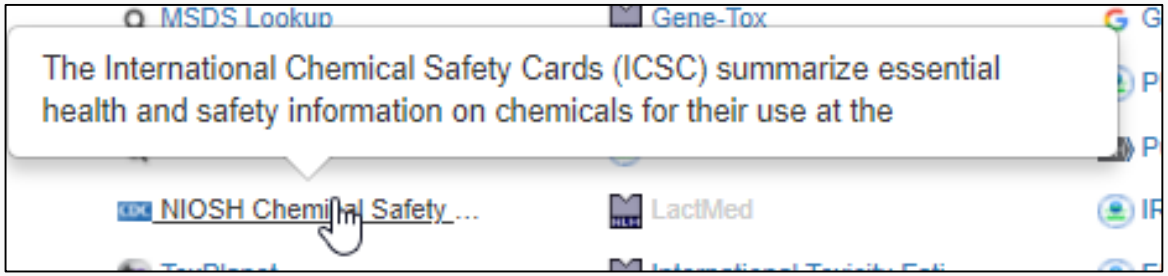
- FOR-IDENT
- NEMI: National Environmental Methods Index
- RSC Analytical Abstracts
- Tox21 Analytical Data
- MONA: MassBank North America
- mzCloud
- NIST IR Spectrum
- NIST MS Spectrum

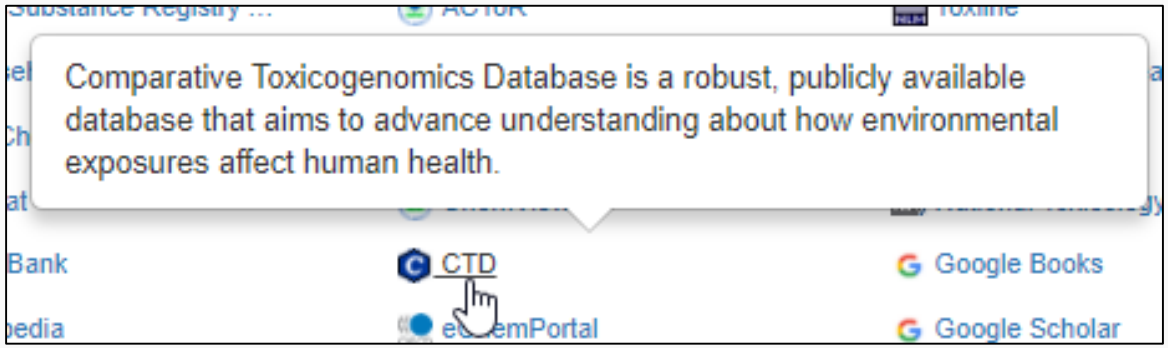
Prediction

- 2D NMR HSQC/HMBC Prediction
- Carbon-13 NMR Prediction
- Proton NMR Prediction
- ChemRTP Predictor
- LSERD

Integrated Linkouts







Integrated Linkouts

Comparative Toxicogenomics DB

EPA United States Environmental Protection Agency

ctd *Illuminating how chemicals affect human health.*

Comparative Toxicogenomics Database

YOUR QUERIES | CONTACT US

Chemicals | Name, CAS RN, ID | Search

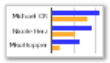
Home | Search | Analyze | Download | Help

Propylene Glycol

Basics | Gene Interactions | Genes | Diseases | Phenotypes | Comps | Pathways | GO | Exposure Studies | Exposure Details | References

These diseases are associated with *Propylene Glycol* or its descendants. Each association is *curated* (M *marker/mechanism* and/or T *therapeutic*) and/or *inferred* (via a curated gene interaction).

Disease categories [Show chart]



Filter by Disease category: ALL | Association type: ALL | Filter

1–50 of 240 results.

First | Previous | 1 | 2 | 3 | 4 | 5 | Next | Last

	Chemical	Disease	Direct Evidence	Enrichment Analysis	Inference Network	Inference Score	References
1.	Propylene Glycol	Drug-Related Side Effects and Adverse Reactions	M	GO	*2 genes:* ABCC2 | ABCC4	4.09	5
2.	Propylene Glycol	Acute Kidney Injury	M	GO	*2 genes:* IL6 | TGFB1	3.78	3
3.	Propylene Glycol	Chemical and Drug Induced Liver Injury	M	GO	*2 genes:* ABCC2 | IL6	2.82	5
4.	Propylene Glycol	Kidney Diseases	M		*1 gene:* TGFB1	2.54	4

Mass and Formula Searches Supporting Mass Spectrometry

EPA United States Environmental Protection Agency

Advanced Search

Mass Search

± | Min/Max

Select Adduct: Neutral

Mass Da ± Error Da Da ppm Search

Molecular Formula Search

Molecular Formula

MS Ready Formula

Exact Formula

Search

Generate Molecular Formula(e)

± | Min/Max

Mass Da ± Error Da ppm Search

Default Options: C[1-50] H[0-100] O[0-20] N[0-20] P[0-20] S[0-10]

Include Halogens: F[0-20] Cl[0-20] Br[0-20] I[0-20]

Advanced Searches
Mass Based Search

EPA United States Environmental Protection Agency

Mass Search

± | Min/Max

M

191.131 Da ± 5 Da | ppm

Search

EPA United States Environmental Protection Agency

Home | Advanced Search | Batch Search | Lists | Predictions | Downloads

Share | Search all data

Search Results

Searched by Mass: 191.131 +/- 5.0 ppm.

298 of 298 chemicals visible

Download / Send

Show info: DTXSID × CASRN × TOXCAST × Mass Diff ×

Select all

Sort by: Mass Difference

Filter by: Name or CASRN | Multicomponent Chemicals ×

DEET
DTXSID: DTXSID2021995
CASRN: 134-62-3
TOXCAST: 14/663
Mass Diff: 0.000014

Phendimetrazine
DTXSID: DTXSID1023447
CASRN: 634-03-7
TOXCAST: 0
Mass Diff: 0.000014

N-Butylacetanilide
DTXSID: DTXSID2042197
CASRN: 91-49-6
TOXCAST: 0
Mass Diff: 0.000014

Benzaldehyde, 4-(diethylamino)-2-methyl-
DTXSID: DTXSID4059041
CASRN: 92-14-8
TOXCAST: 0
Mass Diff: 0.000014

Acetanilide, 2',6'-diethyl-
DTXSID: DTXSID90168148
CASRN: 16665-89-7
TOXCAST: 0
Mass Diff: 0.000014

Azetidine, 1,3-dimethyl-3-(m-methoxyp...
DTXSID: DTXSID40173560
CASRN: 19832-26-9
TOXCAST: 0
Mass Diff: 0.000014

Benzamide, N-pentyl-
DTXSID: DTXSID20174196
CASRN: 20308-43-4

p-t-Butylacetanilide
DTXSID: DTXSID80174238
CASRN: 20330-45-4

N,N-Diethylphenylacetamide
DTXSID: DTXSID00179048
CASRN: 2431-96-1

3-(Dimethylamino)-2-methylpropiophen...
DTXSID: DTXSID60180796
CASRN: 26171-50-6

Butyramide, 2-ethyl-2-phenyl-
DTXSID: DTXSID60184653
CASRN: 30568-39-9

1-Heptanone, 1-(4-pyridyl)-
DTXSID: DTXSID40188594
CASRN: 32941-30-3

Batch Searching

- Singleton searches are useful but we work with thousands of chemicals!

- Typical questions
  - What chemicals can I get for 5000 CAS Numbers?
  - Can I get predicted properties for 1000 chemicals?
  - What is the list of chemicals for the formula $C_xH_yO_z$?
  - What is the list of chemicals for a mass +/- error ?
  - Can I get chemical lists in Excel files? In SDF files?

Batch Searching

Batch Search

Step 1 — Step 2 — Step 3 — Step 4 — Step 5 — Step 6

Step Three: Select Download Data or Display Chemicals

Please enter one identifier per line

Select Input Type(s)

- [ ] Identifiers
  - [ ] Chemical Name
  - [ ] CASRN
  - [ ] InChIKey
  - [ ] DSSTox Substance ID
- [ ] InChIKey Skeleton
- [ ] MS-Ready Formula(e)
- [ ] Exact Formula(e)
- [ ] Monoisotopic Mass

emical Data

Enter Identifiers to Search (searches should be limited to <5000 identifiers)

Fuel oil, no. 1
Ethylene oxide
Chloromethane
1-Chloropropan-2-one
n-Hexane
Ammonia
Nickel carbonyl
Phosgene
Potassium cyanide
Chlorodimethylsilane

Batch Searching

EPA United States Environmental Protection Agency

Select Output Format:

Excel

Download

Customize Results

- [ ] Select All
- [ ] Select All in Lists

Chemical Identifiers

- [x] DTXSID
- [x] Chemical Name
- [ ] CAS-RN
- [ ] InChIKey
- [ ] IUPAC Name

Structures

- [ ] Mol File
- [ ] SMILES
- [ ] InChI String
- [ ] MS-Ready SMILES
- [ ] QSAR-Ready SMILES

Intrinsic And Predicted Properties

- [ ] Molecular Formula
- [ ] Average Mass
- [ ] Monoisotopic Mass
- [ ] TEST Model Predictions
- [ ] OPERA Model Predictions

Presence in Lists:

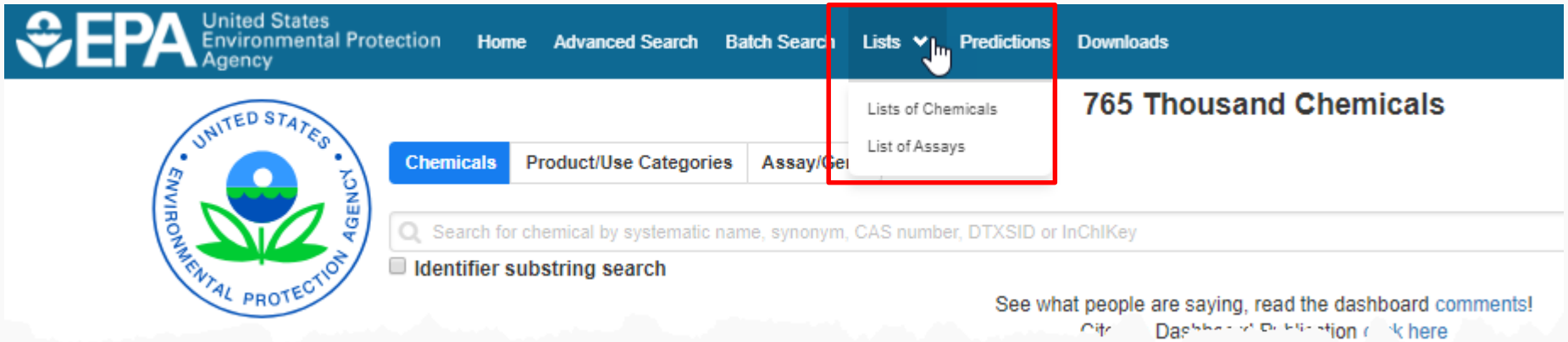
- [ ] ICCVAM test method evaluation report: in vitro ocular toxicity test methods
- [ ] 40CFR355
- [ ] A list of all PBDEs (Polybrominated diphenyl ethers)
- [ ] A list of all PCBs (Polychlorinated biphenyls)
- [ ] A list of polycyclic aromatic hydrocarbons
- [ ] Acute exposure guideline levels
- [ ] Algal Toxins
- [ ] Androgen Receptor Chemicals
- [ ] APCRA Chemicals for Prospective Analysis
- [ ] APCRA Chemicals for Retrospective Analysis
- [ ] APCRA Chemicals for Retrospective Analysis_App_List_448_Chemicals
- [ ] ATSDR Minimal Risk Levels (MRLs) for Hazardous Substances
- [ ] ATSDR Toxic Substances Portal Chemical List
- [ ] Bisphenol Compounds
- [ ] California Office of Environmental Health Hazard Assessment
- [ ] Chemicals with interesting names
- [ ] CMAP
- [ ] DNT Screening Library
- [ ] Drinking Water Suspects, KWR Water, Netherlands
- [ ] EDSP Universe
- [ ] EPA Chemicals associated with hydraulic fracturing

Excel Output

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

Lists of Lists

- Lists of chemicals – ca. 100 lists
- List of ToxCast/Tox21 assays



11 PFAS Lists

http://comptox-prod.epa.gov/dashboard/chemical_lists

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Select List

Download

Show 10 entries

Search: pfas

List Acronym	List Name	Last Updated	Number of Chemicals	List Description
EPAPFAS75S1	EPA PFAS List of 75 Test Samples (Set 1)	2018-06-29	74	PFAS list corresponds to 75 samples (Set 1) submitted for initial testing screens conducted by EPA researchers in collaboration with researchers at the National Toxicology Program.
EPAPFASCAT	Registered DSSTox "category substances" representing Per- and Polyfluoroalkyl Substances (PFAS) categories	2018-06-29	64	List of registered DSSTox "category substances" representing PFAS categories created using ChemAxon's Markush structure-based query representations.
EPAPFASINSOL	PFAS in EPA's Chemical Inventory Insoluble in DMSO	2018-06-29	43	PFAS chemicals included in EPA's expanded ToxCast chemical inventory found to be insoluble in DMSO above 5mM.
EPAPFASINV	PFAS in EPA's ToxCast Chemical Inventory	2018-06-29	430	PFAS chemicals included in EPA's expanded ToxCast chemical inventory and available for testing.
EPAPFASRL	EPA PFAS Cross-Agency Research List	2018-07-27	194	EPAPFASRL is a manually curated listing of mainly straight-chain and branched PFAS (Per- & Poly-fluorinated alkyl substances) compiled from various internal, literature and public sources by EPA researchers and program office representatives.
PFASEPA	PFAS_EPA List of Perfluorinated alkyl substances	2017-11-03	190	PFAS_EPA (Perfluorinated alkyl substances) is a manually curated listing of mainly straight-chain and branched PFAS substances
PFASEUOECD	PFAS Listed in OECD Global Database	2018-07-26	4725	OECD released a New Comprehensive Global Database of Per- and Polyfluoroalkyl Substances, (PFASs)listing approximately 4700 new PFAS
PFASGRACE	PFASforGrace	2017-02-16	35	A list of polyfluorinated chemicals of interest to Grace Patlewicz
PFASKEMI	PFAS List from the Swedish Chemicals Agency (KEMI) Report	2017-02-09	2397	Perfluorinated substances from a Swedish Chemicals Agency (KEMI) Report on the occurrence and use of highly fluorinated substances.
PFASMASTER	PFAS Master List of PFAS Substances	2018-07-26	5061	PFASMASTER is a consolidated list of PFAS substances spanning and bounded by the below lists of current interest to researchers and regulators worldwide.

Showing 1 to 10 of 11 entries (filtered from 96 total entries)

The OECD List of PFAS

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

The OECD releases a new list of PFASs

The OECD releases a new list of Per- and Polyfluoroalkyl Substances (PFASs) based on a comprehensive analysis of information available in the public domain. In total, 4730 PFAS-related CAS numbers have been identified and categorised in this study, including several new groups of PFASs that fulfil the common definition of PFASs (i.e. they contain at least one perfluoroalkyl moiety) but have not yet been commonly regarded as PFASs.

This work has been conducted under the OECD/UN Environment Global PFC Group in support of the Strategic Approach to International Chemicals Management (SAICM) and shifting to safer alternatives for PFASs.

The New Comprehensive Global Database of Per- and Polyfluoroalkyl Substances (PFASs) comes with a methodology report also detailing the major findings with respect to the total numbers and types of PFASs identified, the limitations, gaps and challenges identified in the development of the new list, and opportunities for improving the future understanding of PFASs production, use on the global market, and presence in the environment, biota, and other matrices.

The OECD List of PFAS

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

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PFAS Listed in OECD Global Database

Search PFASEUOECD Chemicals

Substring search

List Details

Description: OECD released a New Comprehensive Global Database of Per- and Polyfluoroalkyl Substances (PFASs) listing approximately 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: 4725

4725 chemicals

Download / Send | **Show info:** DTXSID × CASRN × TOXCAST × | Select all

Sort by: DTXSID | **Filter by:** Name or CASRN | Hide

List of Assays

EPA United States Environmental Protection Agency

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Assay List

Download | Search by Name or Gene

Assay Component Endpoint Name	Details	Active Hits	Description	Gene Symbol
ACEA_T47D_80hr_Negative		469 / 1816	Data from the assay component ACEA_T47D_80hr was analyzed into 2 assay endpoints. This assay endpoint, ACEA_T47D_80hr_Negative, was analyzed in the negative fitting direction relative to DMSO as the negative control and baseline of activity. Using a type of growth reporter, loss-of-signal activity can be used to understand changes in the viability. Furthermore, this assay endpoint can be referred to as a secondary readout, because this assay has produced multiple assay endpoints where this one serves a viability function. To generalize the intended target to other relatable targets, this assay endpoint is annotated to the 'cell cycle' intended target family, where the subfamily is 'cytotoxicity'.	
ACEA_T47D_80hr_Positive		311 / 1816	Data from the assay component ACEA_T47D_80hr was analyzed into 2 assay endpoints. This assay endpoint, ACEA_T47D_80hr_Positive, was analyzed in the positive fitting direction relative to DMSO as the negative control and baseline of activity. Using a type of growth reporter, measures of the cells for gain-of-signal activity can be used to understand the signaling at the pathway-level as they relate to the gene ESR1. Furthermore, this assay endpoint can be referred to as a primary readout, because this assay has produced multiple assay endpoints where this one serves a signaling function. To generalize the intended target to other relatable targets, this assay endpoint is annotated to the 'nuclear receptor' intended target family, where the subfamily is 'steroidal'.	ESR1
APR_HepG2_CellCycleArrest_1h_dn		3 / 310	Data from the assay component APR_HepG2_CellCycleArrest_1hr was analyzed into 2 assay endpoints. This assay endpoint, APR_HepG2_CellCycleArrest_1h_dn, was analyzed in the negative fitting direction relative to DMSO as the negative control and baseline of activity. Using a type of morphology reporter, measures of all nuclear dna for loss-of-signal activity can be used to understand the signaling at the pathway-level as they relate to the gene . Furthermore, this assay endpoint can be referred to as a primary readout, because this assay has produced multiple assay endpoints where this one serves a signaling function. To generalize the	

Select an Assay to Navigate Tile View

EPA United States Environmental Protection Agency

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Assay Endpoint Name: ACEA_T47D_80hr_Positive

Assay Details

Assay Endpoint Name: ACEA_T47D_80hr_Positive

Assay Source Description: ACEA Biosciences, Inc. (ACEA) is a privately owned biotechnology company that developed a real-time, label-free, cell-based assay system based on a microelectronic readout called xCELLigence.

311 of 1813 chemicals visible

Download / Send | Show info: DTXSID × PubChem × CASRN × | Select all

Sort by: DTXSID | Filter by: Name or CASRN | Inactive ×

Sodium L-ascorbate
DTXSID: DTXSID0020105
PubChem: 41
CASRN: 134-03-2

Benzyl acetate
DTXSID: DTXSID0020151
PubChem: 101
CASRN: 140-11-4

2,4-Dinitrophenol
DTXSID: DTXSID0020523
PubChem: 154
CASRN: 51-28-5

17beta-Estradiol
DTXSID: DTXSID0020573
PubChem: 351
CASRN: 50-28-2

Mestranol
DTXSID: DTXSID0020814
PubChem: 97
CASRN: 72-33-3

Select an Assay to Navigate Table View

EPA United States Environmental Protection Agency

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

Assay Endpoint Name: ACEA_T47D_80hr_Positive

Assay Details

Assay Endpoint Name: ACEA_T47D_80hr_Positive

Assay Source Description: ACEA Biosciences, Inc. (ACEA) is a privately owned biotechnology company that developed a real-time, label-free, cell-based assay system based on a microelectronic readout called xCELLigence.

311 of 1813 chemicals visible

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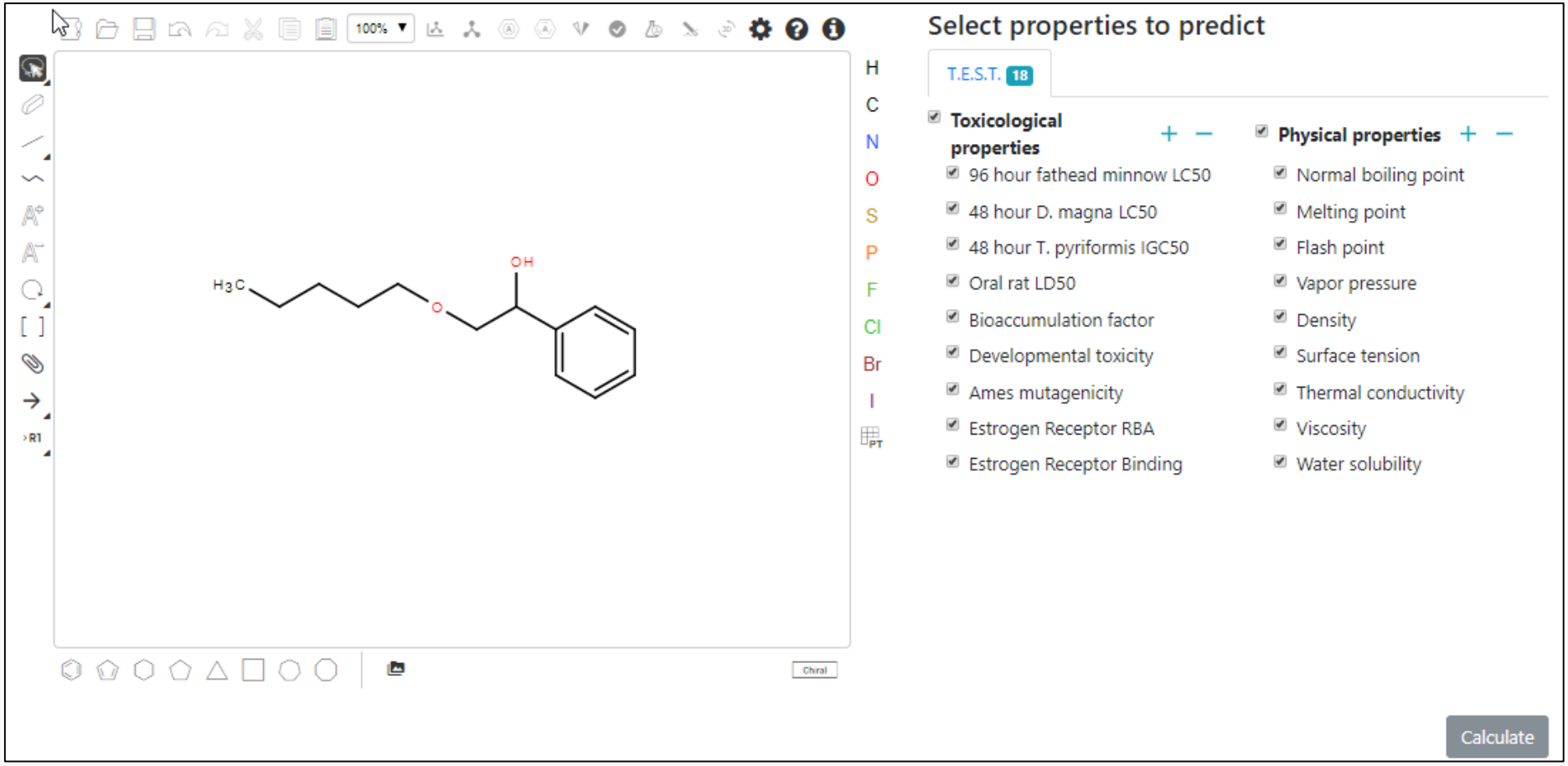
Sort by: DTXSID | Filter by: Name or CASRN | Inactive ×

Structure	DTXSID	Preferred Name	# ToxCast Active	% ToxCast Active	Hit Call	Top	Scaled Top	AC50 (uM)	logAC50 (uM)
	DTXSID9047542 ToxCast™	Picoxystrobin	127/558	23%	Active	56.0	2.30	10.9	1.04
	DTXSID9047255 ToxCast™	CP-465394	16/538	3%	Active	30.1	1.24	82.2	1.91
	DTXSID9047178 ToxCast™	2-Ethylhexyl octadecanoate	10/469	2%	Active	24.8	1.02	20.7	1.32

Real-Time Predictions



Real-Time Predictions

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

Downloadable Data Being Updated

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Chemistry Dashboard

Downloads

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        DTXSID
316388891  20404      DTXSID30873143
316388890  10142816   DTXSID70873142
316388889  50742127   DTXSID40873139
316388888  19073841   DTXSID20873137
316388887  11505215   DTXSID00873135
316388886  25021861   DTXSID80873133
316388885  2784427    DTXSID60873131
316388884  6731       DTXSID00873130
```

DSSTox identifiers mapped to CAS Numbers and Names File — Posted: 11/14/2016

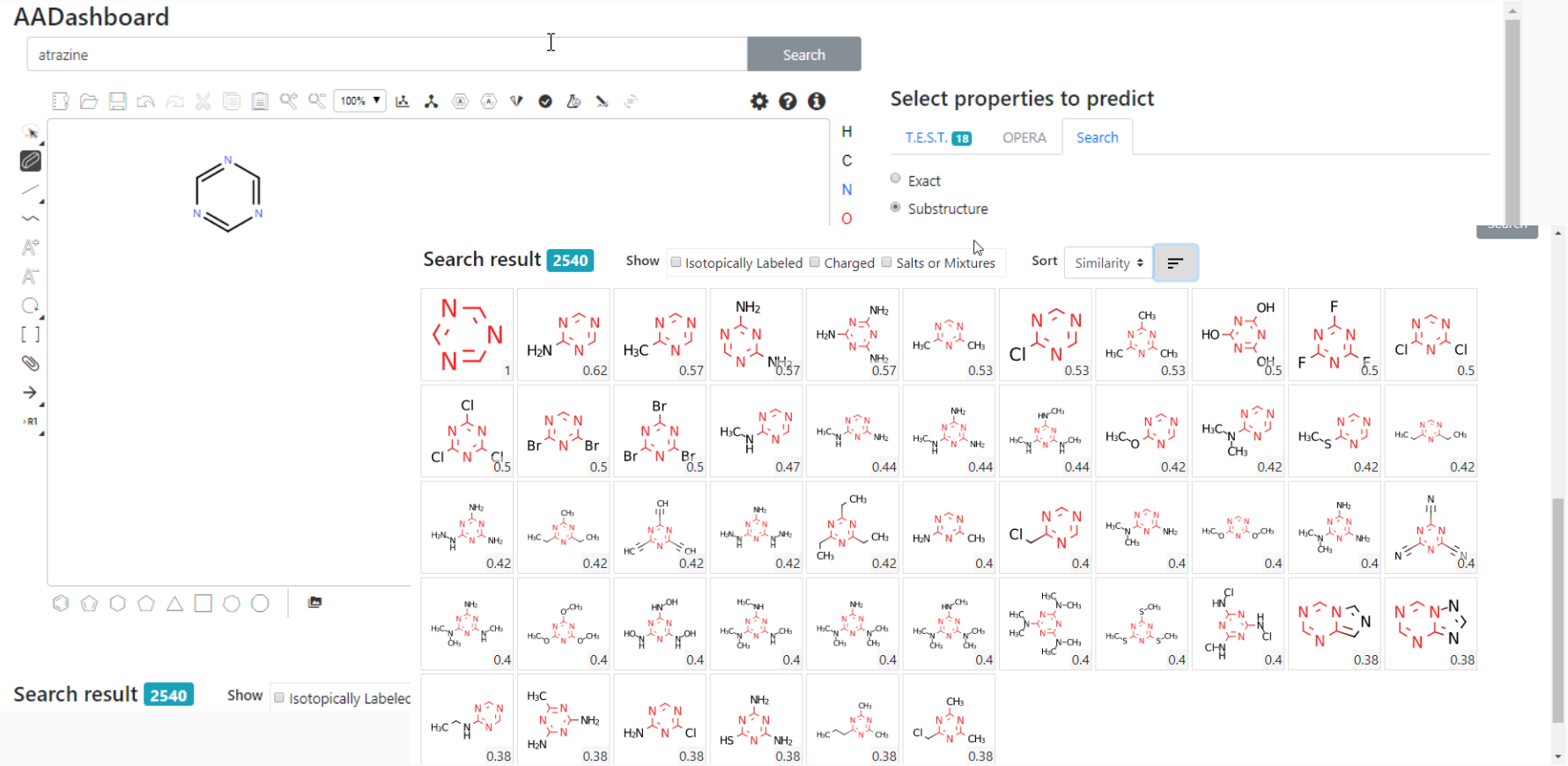
The DSSTox Identifiers file is in Excel format and includes the CAS Number, DSSTox substance identifier (DTXSID) and the Preferred Name.

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) phenylhydrazine

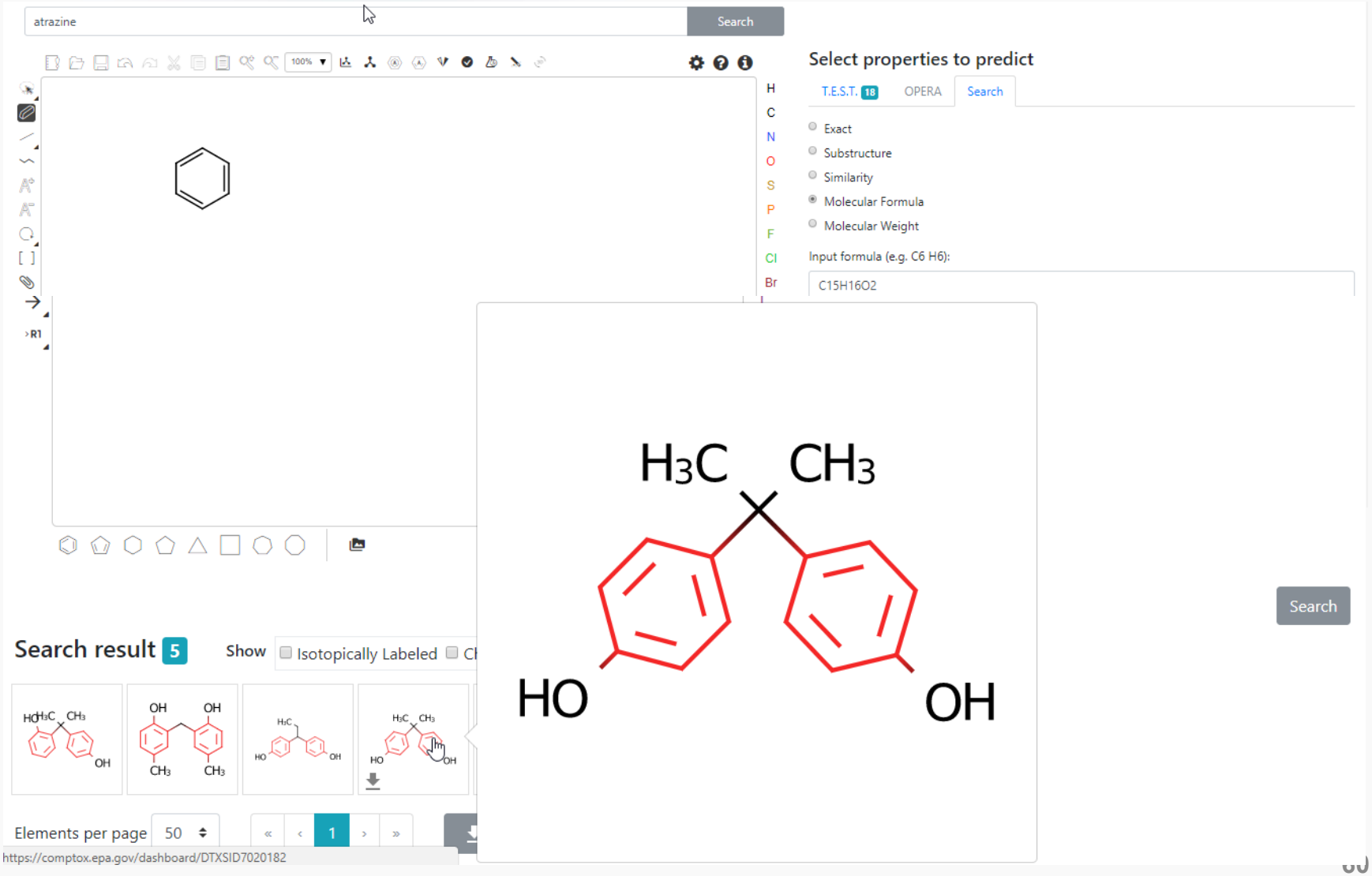
Work in Progress "InvitroDB_v3"

- The last public release of ToxCast data (invitroDB_v2) was in 3rd Quarter of 2015
- The next release invitroDB_v3 is Fall 2018
- Data includes new assays, new chemicals, new pipelining, results of data curation
- Data will also release via the Dashboard
- Data will be available at https://www.epa.gov/chemical-research/exploring-toxcast-data-downloadable-data

Prototype Development

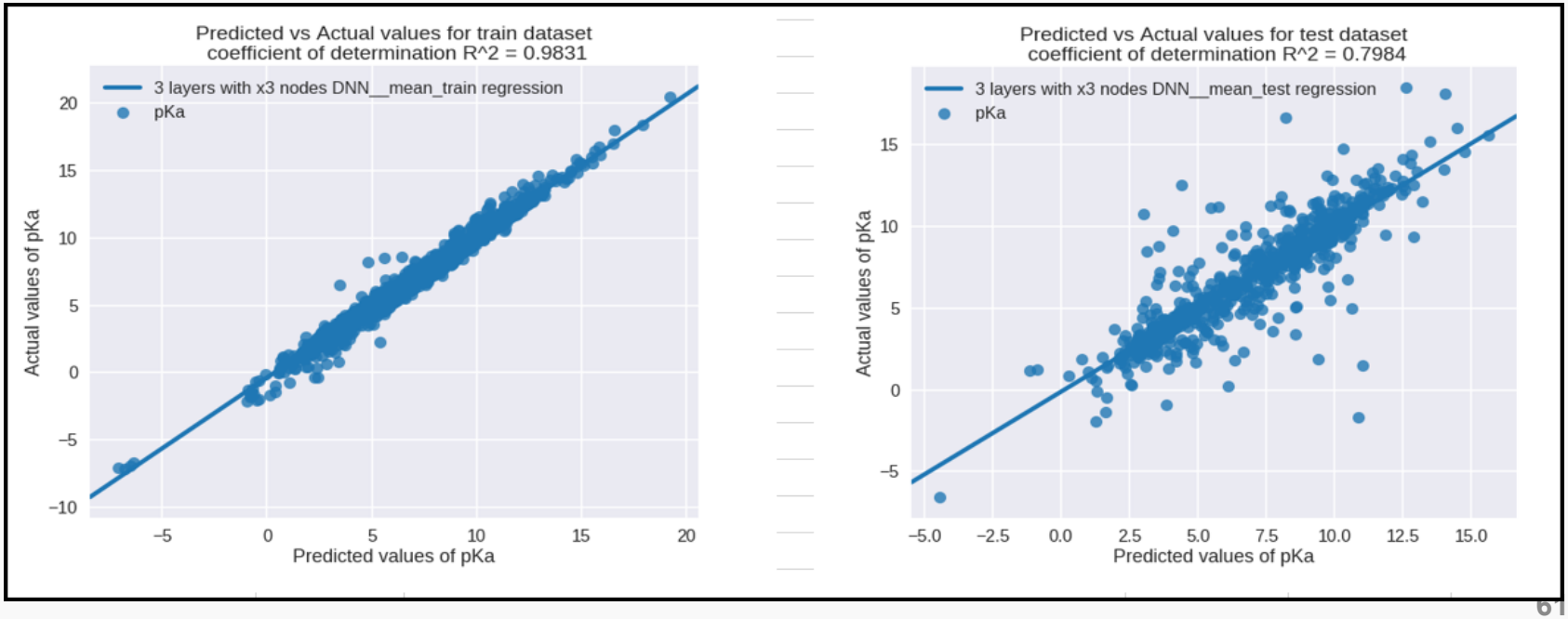


Prototype Development



pKa Prediction Model

- pKa prediction models based on Open Data Set of 8000 chemicals – acidic, basic and amphoteric chemicals



Conclusion

- The CompTox Chemistry Dashboard provides access to data for ~765,000 chemicals
- An expanding list of data types and sources has been integrated
- New searches based on Product Use and Categories and Assay and Gene
- The chemical lists of interest grows with each release

- Next release scheduled for Fall 2018 with InvitroDB_v3 data – more chemicals, more assays

Acknowledgements

<u>EPA-RTP</u>

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NHERL
NRMRL

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Journal of Cheminformatics

DATABASE Open Access

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

Antony J. Williams[1*], Christopher M. Grulke[1], Jeff Edwards[1], Andrew D. McEachran[2], Kamel Mansouri[1,2,4], Nancy C. Baker[3], Grace Patlewicz[1], Imran Shah[1], John F. Wambaugh[1], Richard S. Judson[1] and Ann M. Richard[1]

https://doi.org/10.1186/s13321-017-0247-6