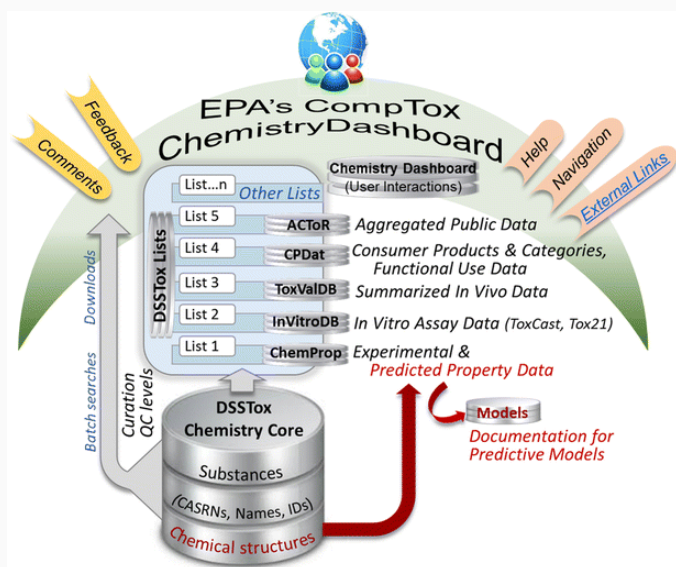


# The EPA Comptox Chemistry Dashboard: A Web-Based Data Integration Hub for Environmental Chemistry and Toxicology Data



**Antony Williams**

*U.S. Environmental Protection Agency, RTP, NC*

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

- A new architecture bringing together all data
- A **publicly accessible website** delivering access:
  - ~760,000 chemicals with related property data
  - Experimental and predicted physicochemical property data
  - Experimental Human and Ecological hazard data
  - Integration to “biological assay data” for 1000s of chemicals
  - Information regarding consumer products containing chemicals
  - Links to other agency websites and public data resources
  - “Literature” searches for chemicals using public resources
  - “Batch searching” for thousands of chemicals
  - Real time prediction of physchem and toxicity endpoints

# CompTox Chemistry Dashboard

<https://comptox.epa.gov/dashboard>



Home

Advanced Search

Batch Search

Lists

Predictions

Downloads

## Chemistry Dashboard

Aa Aa Aa



761 Thousand Chemicals

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



☐ Identifier substring search



See what people are saying, read the dashboard [comments!](#)

## Latest News

[Read more news](#)

### A Movie Regarding how to Identify "Known Unknowns" Using the CompTox Dashboard

March 28th, 2017 at 7:35:41 PM

Recently we published a paper regarding [Identifying known unknowns using the US EPA's CompTox Chemistry Dashboard](#), *Analytical and Bioanalytical Chemistry*, March 2017, Volume 409, Issue 7, pp 1729–1735. A movie explaining the paper in full animated detail has been put on YouTube. Enjoy the movie interlude [here](#).



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# Detailed Chemical Pages



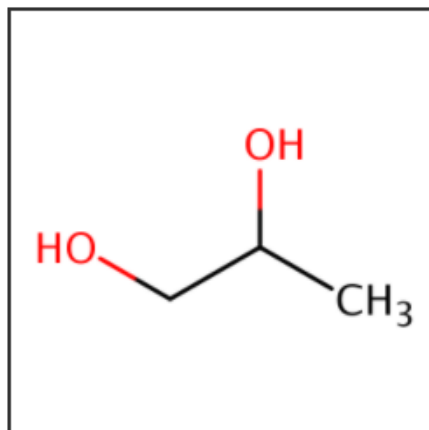
## Chemistry Dashboard | EPAHFR

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### 1,2-Propylene glycol

57-55-6 | DTXSID0021206

© Searched by DSSTox\_Substance\_Id: Found 1 result for 'DTXSID0021206'.



#### Wikipedia

Propylene glycol (IUPAC name: propane-1,2-diol) is a synthetic organic compound with the chemical formula C<sub>3</sub>H<sub>8</sub>O<sub>2</sub>. It is a viscous colorless liquid which is nearly odorless but possesses a faintly sweet taste. Chemically it is classed as a diol and is miscible with a broad range of solvents, including water, acetone, and chloroform. It is produced on a large scale and is primarily used in the production of polymers, but also sees use in food...[Read more](#)

#### Intrinsic Properties

#### Structural Identifiers

#### Linked Substances

#### Presence in Lists

#### Record Information


#### Quality Control Notes

[Executive Summary \(Beta\)](#)[Chemical Properties](#)[Env. Fate/Transport](#)[Hazard](#)[ADME \(Beta\)](#)[Exposure](#)[Bioassays](#)[Similar Compounds](#)[Related Substances](#)[Synonyms](#)[Literature](#)[Links](#)[Comments](#)

# The Executive Summary



# Properties, Fate and Transport

 EPA  
United States  
Environmental Protection  
Agency

HomeAdvanced SearchBatch SearchListsPredictionsDownloads

Search All Data

Chemistry Dashboard

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Download as: TSVExcelSDF

Summary

LogP: Octanol-Water

Water Solubility

Density

Flash Point

Melting Point

Boiling Point

Surface Tension

Thermal Conductivity

Vapor Pressure

Viscosity

LogKoa: Octanol-Air

Henry's Law

Index of Refraction

Molar Refractivity

Molar Volume

| Property             | Average      |              | Median       |           | Range        |                      | Unit              |
|----------------------|--------------|--------------|--------------|-----------|--------------|----------------------|-------------------|
|                      | Experimental | Predicted    | Experimental | Predicted | Experimental | Predicted            |                   |
| LogP: Octanol-Water  | -0.920 (1)   | -0.983 (5)   | -            | -0.966    | -0.920       | -1.34 to -0.780      | -                 |
| Water Solubility     | 13.1 (1)     | 12.6 (4)     | -            | 11.2      | 13.1         | 4.32 to 23.6         | mol/L             |
| Density              | -            | 1.02 (2)     | -            | 1.02      | -            | 1.01 to 1.04         | g/cm <sup>3</sup> |
| Flash Point          | -            | 88.8 (2)     | -            | 88.8      | -            | 70.4 to 107          | °C                |
| Melting Point        | -60.0 (6)    | -30.6 (4)    | -60.0        | -29.3     | -60.0        | -42.4 to -21.6       | °C                |
| Boiling Point        | 187 (6)      | 180 (5)      | 187          | 185       | 187 to 188   | 155 to 200           | °C                |
| Surface Tension      | -            | 35.5 (2)     | -            | 35.5      | -            | 33.1 to 38.0         | dyn/cm            |
| Thermal Conductivity | -            | 185 (1)      | -            | -         | -            | -                    | mW/(m*K)          |
| Vapor Pressure       | 1.29e-01 (1) | 1.91e-01 (4) | -            | 2.08e-01  | 1.29e-01     | 5.37e-02 to 2.95e-01 | mmHg              |
| Viscosity            | -            | 12.6 (1)     | -            | -         | -            | -                    | cP                |
| LogKoa: Octanol-Air  | -            | 6.74 (1)     | -            | -         | -            | -                    | -                 |
| Henry's Law          | -            | 6.02e-08 (1) | -            | -         | -            | -                    | atm-m3/mole       |
| Index of Refraction  | -            | 1.43 (1)     | -            | -         | -            | -                    | -                 |
| Molar Refractivity   | -            | 19.0 (1)     | -            | -         | -            | -                    | cm <sup>3</sup>   |
| Molar Volume         | -            | 73.4 (1)     | -            | -         | -            | -                    | cm <sup>3</sup>   |
| Polarizability       | -            | 7.52 (1)     | -            | -         | -            | -                    | Å <sup>3</sup>    |

Executive Summary (Beta)Chemical PropertiesEnv. Fate/TransportHazardADME (Beta)ExposureBioassaysSimilar CompoundsRelated SubstancesSynonymsLiteratureLinksComments

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

 Journal of Cheminformatics

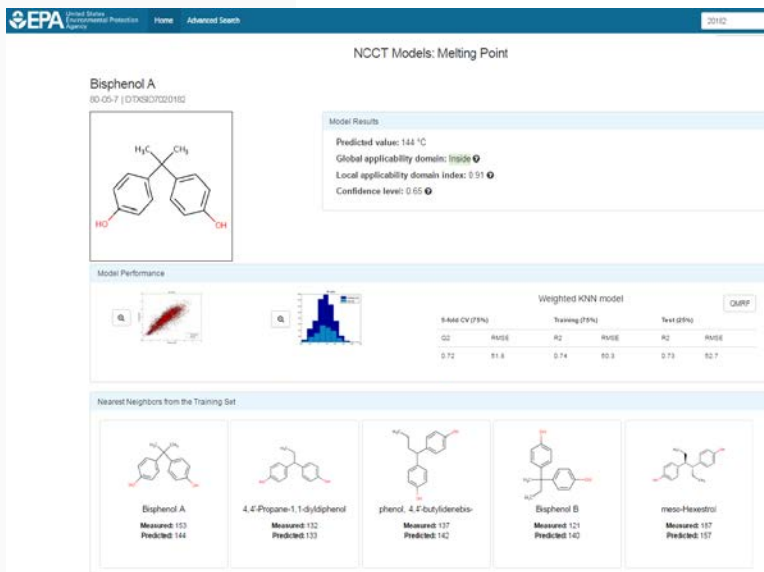
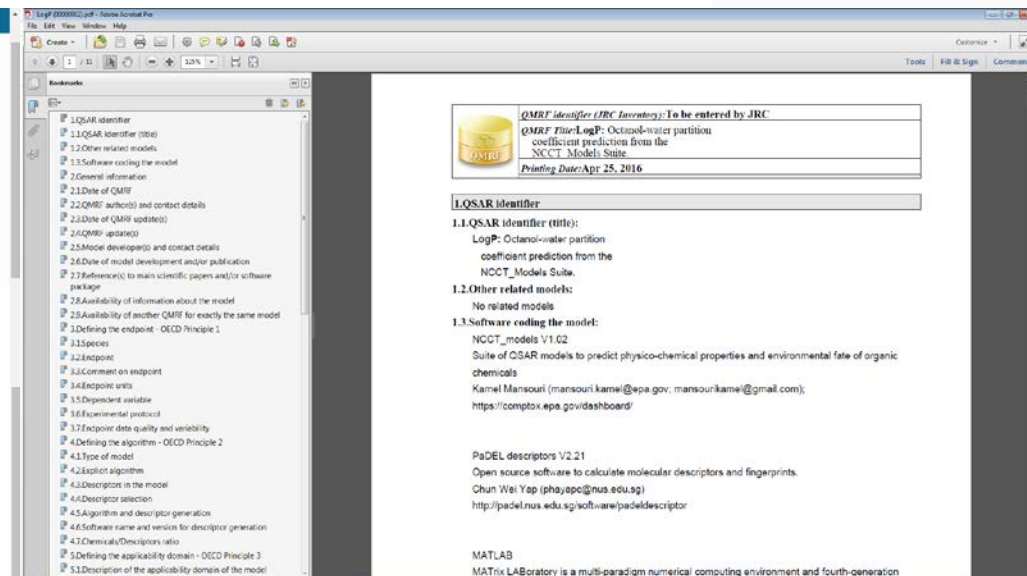
## RESEARCH ARTICLE

Open Access



# OPERA models for predicting physicochemical properties and environmental fate endpoints

Kamel Mansouri<sup>1,2,3\*</sup> , Chris M. Grulke<sup>1</sup>, Richard S. Judson<sup>1</sup> and Antony J. Williams<sup>1</sup>

**QMRP identifier (JRC Inventory): To be entered by JRC**

**QMRP Title:** LogP: Octanol-water partition coefficient prediction from the NCCT Models Suite  
**Printing Date:** Apr 25, 2016

**LogP identifier**

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

**1.2.Other related models:**  
No related models

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

**PaDEL descriptors V2.21**  
Open source software to calculate molecular descriptors and fingerprints.  
Chun Wei Yap (yapcwc@nus.edu.sg)  
<http://padel.nus.edu.sg/software/padeldescriptor>

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



# Access to Chemical Hazard Data



## Chemistry Dashboard | EPAHFR

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Download table as:

[TSV](#)[Excel](#)[Human](#)[Eco](#)

|   | Priority | Type | Subtype     | Risk Assessment Class | Values | Units     | Study Type | Exposure Route | Species | Subsource | Source      |
|---|----------|------|-------------|-----------------------|--------|-----------|------------|----------------|---------|-----------|-------------|
| + | 8        | NOEL | Cardiova... | subchronic            | 5000.0 | mg/kg-day | subchronic | oral           | rat     | Vaill...  | PPRTV (...) |
| + | 8        | NOEL | Endocrine   | subchronic            | 5000.0 | mg/kg-day | subchronic | oral           | rat     | Vaill...  | PPRTV (...) |
| + | 8        | LOEL | Hematol...  | subchronic            | 2500.0 | mg/kg-day | subchronic | oral           | rat     | Vaill...  | PPRTV (...) |
| + | 8        | LOEL | Hepatic     | subchronic            | 2500.0 | mg/kg-day | subchronic | oral           | rat     | Vaill...  | PPRTV (...) |
| + | 8        | NOEL | Immune      | immunot...            | 5000.0 | mg/kg-day | subchronic | oral           | rat     | Vaill...  | PPRTV (...) |
| + | 8        | NOEL | Renal       | subchronic            | 5000.0 | mg/kg-day | subchronic | oral           | rat     | Vaill...  | PPRTV (...) |
| + | 8        | LOEL | Systemic    | subchronic            | 2500.0 | mg/kg-day | subchronic | oral           | rat     | Vaill...  | PPRTV (...) |
| + | 8        | NOEL | Hematol...  | subchronic            | 1500.0 | mg/kg-day | subchronic | oral           | rabbit  | Vaill...  | PPRTV (...) |
| + | 8        | NOEL | Systemic    | subchronic            | 1500.0 | mg/kg-day | subchronic | oral           | rabbit  | Vaill...  | PPRTV (...) |

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# Product Composition Details

Product & Use Categor...

Chemical Weight Fra...

Chemical Functional Use

Monitoring Data

Exposure Predictions

Chemical Weight Fractions 

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

Chemical Properties

Env. Fate/Transport

Toxicity Values (Beta)

ADME (Beta)

Exposure

Bioassays

Similar Molecules (Beta)

Synonyms

Literature

External Links

# In Vitro Bioassay Screening

## ToxCast and Tox21

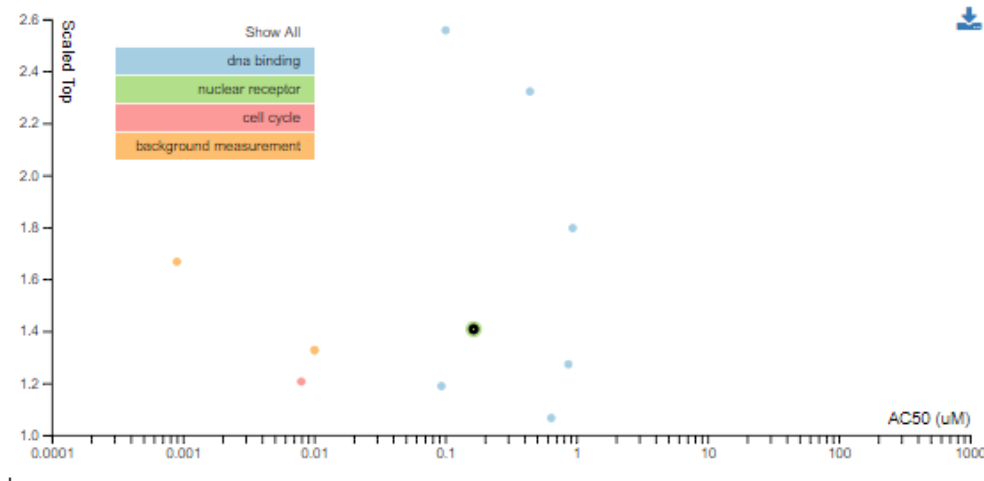


## Chemistry Dashboard | EPAHFR

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### Chemical Activity Summary

#### ToxCast Data



#### Assay Details

AC50 (uM): 0.16  
Scaled top: 1.41  
Assay Name: NVS\_NR\_hFXR\_Antagonist  
**Assay Description: 716**  
Gene Symbol: NR1H4  
Organism: human  
Tissue: NA  
Assay Format Type: biochemical  
Biological Process Target: receptor binding  
Detection Technology: TR-FRET  
Analysis Direction: positive  
Intended Target Family: nuclear receptor  
Description: Data from the assay component NVS\_NR\_hFXR\_Antagonist was analyzed into 1 assay endpoint. This assay endpoint, NVS\_NR\_hFXR\_Antagonist, was analyzed in the positive fitting direction relative to DMSO as the negative control and baseline of activity. Using a type of binding reporter, loss-of-signal activity can be used to understand changes in the binding as they relate to the gene NR1H4.

[Assay Name](#)[Assa...](#)[SeqA...](#)[AOP Link](#)[AOP Eve...](#)[Hit Call...](#)[T...](#)[Scale...](#)[log ...](#)[Target Family](#)[Executive Summary \(Beta\)](#)[Chemical Properties](#)[Env. Fate/Transport](#)[Hazard](#)[ADME \(Beta\)](#)[Exposure](#)[Bioassays](#)[Similar Compounds](#)[Related Substances](#)[Synonyms](#)[Literature](#)[Links](#)[Comments](#)

# Detailed Assay Description as PDF (limited number of assays)

NVS\_NR\_hFXR\_Antagonist

**Assay Title: NovaScreen Human Farnesoid x Receptor Alpha (FXR) Ligand-Binding Antagonist Screening Assay**

## 1. Assay Descriptions

### 1.1. Overview

#### Assay Summary:

High-throughput screening of in vitro chemical-target interactions across a wide variety of compounds through a broad range of biochemical interactions will help describe the chemical-assay bioactivity space for chemicals with limited available information. There exists a large number of environmental chemicals for which there is little information about the potential for bioactivity. The NVS NR human farnesoid x receptor (FXR, NR1H4) agonist assay format allows for an efficient screening of thousands of chemicals for the ability to competitively bind to the ligand-binding domain of a xenobiotic sensing nuclear receptor. This assay was developed to screen the ToxCast chemical library for potential farnesoid x receptor ligand-binding activity using a TR-FRET competitive displacement assay and a known FXR receptor agonist (Chenodeoxycholic Acid, CDCA) as a reference compound. Biochemical high-throughput screening offers preliminary evidence for chemical targets in a cell or tissues which, when combined with information from literature or targeted in vivo studies, can indicate potential pathways for toxicity. This assay was run for a test duration of 1 hour in a 384-well plate.















### 1.2. Assay Definition

#### Assay Throughput:

Human FXR ligand-binding domain (LBD) incubated in 384-well microtiter plates for 1 hour prior to measuring ligand dependent binding of cofactor to the receptor using TR-FRET.

# The Assay Table

Download as: [TSV](#) [Excel](#) Show: [Inactive](#) [Background](#)

| Assay Name  | Assay De... |  SeqAPASS                    | AOP Link ↑ | AOP Event Link |  Hit Call |  Top | Scaled Top |  AC50 | log AC50 |  Target Family |
|---|-------------|---|------------|----------------|--|---|------------|--|----------|---|
|  CEETOX_H295R ESTRONE_up | 909         | -   | -          | -              | ACTIVE   | 1.24  | 1.53       | 1.06   | 0.0236   | steroid hormone   |
|  ATG_PXR_TRANS_up        | -           | <a href="#">NP_071285.1</a>  | 60         | 245            | ACTIVE   | 1.89  | 1.43       | 21.3   | 1.33     | nuclear receptor  |
|  NVS_GPCR_hH1            | -           | <a href="#">NP_000852.1</a>  | -          | -              | ACTIVE   | 21.2  | 1.06       | 1.42   | 0.151    | gpcr  |
|  NVS_GPCR_hAdoRA2a       | -           | <a href="#">NP_000666.2</a>  | -          | -              | ACTIVE   | 26.2  | 1.05       | 6.95   | 0.842    | gpcr  |
|  NVS_GPCR_hAdoRA1        | -           | <a href="#">NP_000665.1</a>  | -          | -              | ACTIVE   | 53.5  | 1.97       | 6.44   | 0.809    | gpcr  |

# Single Click Download

|    | A                                 | B                 | C              | D        | E              | F        | G     | H         | I        | J       | K                      | L | M |
|----|-----------------------------------|-------------------|----------------|----------|----------------|----------|-------|-----------|----------|---------|------------------------|---|---|
| 1  | Assay Name                        | Assay Description | SeqAPASS       | AOP Link | AOP Event Link | Hit Call | Top   | Scaled To | AC50     | logAC50 | Intended Target Family |   |   |
| 2  | ATG_TCF_b_cat_CIS_dn              | -                 | -              | -        | -              | ACTIVE   | 0.872 | 1.27      | 0.869    | -0.0609 | dna binding            |   |   |
| 3  | NVS_NR_hFXR_Antagonist            | 716               | NP_001193922.1 | 61       | 479            | ACTIVE   | 35.6  | 1.41      | 0.165    | -0.783  | nuclear receptor       |   |   |
| 4  | ATG_XTT_Cytotoxicity_up           | -                 | -              | -        | -              | ACTIVE   | 98.7  | 1.21      | 0.00800  | -2.10   | cell cycle             |   |   |
| 5  | ATG_Oct_MLP_CIS_dn                | -                 | -              | -        | -              | ACTIVE   | 0.838 | 1.19      | 0.0936   | -1.03   | dna binding            |   |   |
| 6  | ATG_AP_2_CIS_dn                   | -                 | -              | -        | -              | ACTIVE   | 0.806 | 2.56      | 0.101    | -0.997  | dna binding            |   |   |
| 7  | ATG_M_19_TRANS_up                 | -                 | -              | -        | -              | ACTIVE   | 0.608 | 1.67      | 0.000901 | -3.05   | background measurement |   |   |
| 8  | ATG_M_06_TRANS_dn                 | -                 | -              | -        | -              | ACTIVE   | 0.349 | 1.33      | 0.0101   | -2.00   | background measurement |   |   |
| 9  | ATG_GLI_CIS_dn                    | -                 | -              | -        | -              | ACTIVE   | 0.905 | 2.32      | 0.443    | -0.354  | dna binding            |   |   |
| 10 | ATG_M_61_TRANS_dn                 | -                 | -              | -        | -              | ACTIVE   | 0.349 | 1.33      | 0.0101   | -2.00   | background measurement |   |   |
| 11 | ATG_HIF1a_CIS_dn                  | -                 | -              | -        | -              | ACTIVE   | 1.41  | 1.80      | 0.937    | -0.0282 | dna binding            |   |   |
| 12 | ATG_HNF6_CIS_dn                   | -                 | -              | -        | -              | ACTIVE   | 0.386 | 1.07      | 0.643    | -0.192  | dna binding            |   |   |
| 13 | TOX21_AR_BLA_Agonist_ch1          | -                 | -              | -        | -              | INACTIVE | 0.00  | 0.00      | -        | -       | background measurement |   |   |
| 14 | TOX21_AR_BLA_Agonist_ch2          | -                 | -              | -        | -              | INACTIVE | 0.00  | 0.00      | -        | -       | background measurement |   |   |
| 15 | TOX21_AR_BLA_Agonist_ratio        | 761               | P10275.2       | 187      | 1134           | INACTIVE | 0.00  | 0.00      | -        | -       | nuclear receptor       |   |   |
| 16 | TOX21_AR_BLA_Antagonist_ratio     | 762               | P10275.2       | 187      | 1134           | INACTIVE | 0.00  | 0.00      | -        | -       | nuclear receptor       |   |   |
| 17 | TOX21_AR_BLA_Antagonist_viability | -                 | -              | -        | -              | INACTIVE | 0.00  | 0.00      | -        | -       | cell cycle             |   |   |
| 18 | TOX21_AR_LUC_MDAKB2_Agonist       | 764               | P10275.2       | 187      | 1134           | INACTIVE | 0.00  | 0.00      | -        | -       | nuclear receptor       |   |   |
| 19 | TOX21_AR_LUC_MDAKB2_Antagonist    | 765               | P10275.2       | 187      | 1134           | INACTIVE | 0.00  | 0.00      | -        | -       | nuclear receptor       |   |   |
| 20 | TOX21_Aromatase_Inhibition        | -                 | NP_000094.2    | 153      | 964            | INACTIVE | 0.00  | 0.00      | -        | -       | cyp                    |   |   |
| 21 | TOX21_AutoFluor_HEK293_Cell_blue  | -                 | -              | -        | -              | INACTIVE | 0.00  | 0.00      | -        | -       | background measurement |   |   |

# Literature Searches and Links

## Rebuilt Abstract Sifter

Chemical Properties

Env. Fate/Transport

Hazard

ADME (Beta)

Exposure

Bioassays

Similar Compounds

Related Substances

Synonyms

Literature

Links

Comments

Google Scholar

PubMed Abstract Sifter

PubChem Articles

PubChem Patents

PPRTV

IRIS

Select a Query Term

Select a Query Term

Hazard

Fate and Transport

Metabolism/PK/PD

Chemical Properties

Exposure

Mixtures

Male Reproduction

Androgen Disruption

Female Reproduction

GeneTox

Embryo and embryonic development

Child (infant through adolescent)

Dust and Exposure

before retrieving.

ylene glycol" OR "Propylene Glycol") AND (NOAEL or OR "reference dose" OR "reference concentration" OR b] OR "cancer slope factor"[tiab])

wnload / Send to...














Download Sifter for Excel

| nal  | Rev |
|--|-----|
| ws on environmental health                             |     |
| ation toxicology                                       |     |
| ational journal of hygiene and environmental h...      |     |
| oo induced diseases                                    |     |
| ductive toxicology (Elmsford, N.Y.)                    |     |
| latory toxicology and pharmacology : RTP               |     |
| biotica; the fate of foreign compounds in biolog...    |     |
| ology  |     |
| ational journal of toxicology                          |     |
| analysis : an official publication of the Society f... |     |
| ological sciences : an official journal of the Soc...  |     |














[ptox.zn.epa.gov/dashboard/dsstoxdb/re:](https://ptox.zn.epa.gov/dashboard/dsstoxdb/re:)

# Links to Other Resources











## General

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






## Toxicology

-  ACToR
-  DrugPortal
-  CCRIS
-  ChemView
-  CTD
-  e...
-  E...
-  G...
-  HSDB
-  ToxCast Dashboar...
-  LactMed
-  ACToR PDF Report
-  International Toxicit...

## Publications

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

## Analytical

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

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



- Build out definitive “lists” of chemicals
  - Algal toxins
  - EPA IRIS Chemical List
  - National Environmental Methods Index
  - NIOSH International Safety Cards
  - Pesticides
  - **Toxcast screening chemical collection**

# The Collection of Lists

## Chemistry Dashboard

Aa ▼ Aa ▲

|  |      |  |
|--|------|--|
| Relevant Substances  |      | projects, hosted by IfU, HSWT and TUM. The database at <a href="https://www.lfu.bayern.de/stoffident/#/home">https://www.lfu.bayern.de/stoffident/#/home</a> has additional functionali...                               |
| Superfund Chemical Data Matrix   | 220  | The Superfund Chemical Data Matrix (SCDM) generates a list of the corresponding Hazard Ranking System (HRS) factor values, benchmarks, and data elements for a particular chemical.                                      |
| Surfactant List Screened in Swiss  | 122  | EAWAGSURF is a list of surfactants screened in Swiss wastewater effluents as part of a 2014 study. Structures/mixtures are being   |
| <b>TOXCAS</b> T - EPA <b>ToxCas</b> T Screening Library                            | 4746 | <b>TOXCAS</b> T is the complete list of chemicals having undergone some level of screening in EPA's <b>ToxCas</b> T research program since 2007 (last updated 4/11/2017); sublists included.                             |
| <b>TOXCAS</b> T_e1k - EPA <b>ToxCas</b> T Screening Library (e1k Subset)           | 799  | <b>TOXCAS</b> T_e1k is the e1k subset of <b>TOXCAS</b> T, selected for screening in endocrine-related assays.  |
| <b>TOXCAS</b> T_ph1v2 - EPA <b>ToxCas</b> T Screening Library (ph1v2 Subset)       | 293  | <b>TOXCAS</b> T_ph1v2 is the ph1v2 subset of <b>TOXCAS</b> T, a reprocurd subset of Phase I (ph1v1) chemicals moved into Phase II and later testing phases of the <b>ToxCas</b> T program.                               |
| <b>TOXCAS</b> T_ph2 - EPA <b>ToxCas</b> T Screening Library (ph2 Subset)           | 768  | <b>TOXCAS</b> T_ph2 is the ph2 subset of <b>TOXCAS</b> T, added in Phase II of the <b>ToxCas</b> T program to increase chemical diversity and coverage of chemicals of concern to EPA programs.                          |
| <b>TOXCAS</b> T_ph3 - EPA <b>ToxCas</b> T Screening Library (ph3 subset)           | 2678 | <b>TOXCAS</b> T_ph3 is the ph3 subset of <b>TOXCAS</b> T, added to the most recent Phase III of the <b>ToxCas</b> T program to further increase chemical diversity and coverage of chemicals of concern to EPA programs. |
| <b>TOXCAS</b> T_PhaseI - EPA <b>ToxCas</b> T Screening Library (Phase I subset)    | 310  | <b>TOXCAS</b> T_PhaseI corresponds to the ph1v1 subset of <b>TOXCAS</b> T (mostly pesticides) screened in Phase I of the <b>ToxCas</b> T program.  |
| <b>TOXCAS</b> T_PhaseII - EPA <b>ToxCas</b> T Screening Library (Phase II Subset)  | 1864 | <b>TOXCAS</b> T_PhaseII is the full set of chemicals screened in Phase II of the <b>ToxCas</b> T program, consisting of <b>TOXCAS</b> T_ph1v2, ph2 and e1k sublists.   |
| <b>TOXCAS</b> T_PhaseIII - EPA <b>ToxCas</b> T Screening Library (Phase II Subset) | 4584 | <b>TOXCAS</b> T_PhaseIII is the full set of chemicals available for screening in Phase III of the <b>ToxCas</b> T program, consisting of the majority of chemicals screened in Phase II and newly added ph3 chemicals.   |
| TSCA Surfactant List (subset)  | 100  | TSCASURF contains information on surfactants compiled by James Little (while at Eastman Chemical) from the TSCA Database. This is being progressively curated and extended.  |
| University Jaume I Target Substances   | 508  | UJIBADE is a list of target substances from University Jaume I, Castellon, Spain used for retention time prediction in Bade et al 2015, DOI: 10.1016/j.scitotenv.2015.08.078   |

# ToxCast phases over time

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Perspective

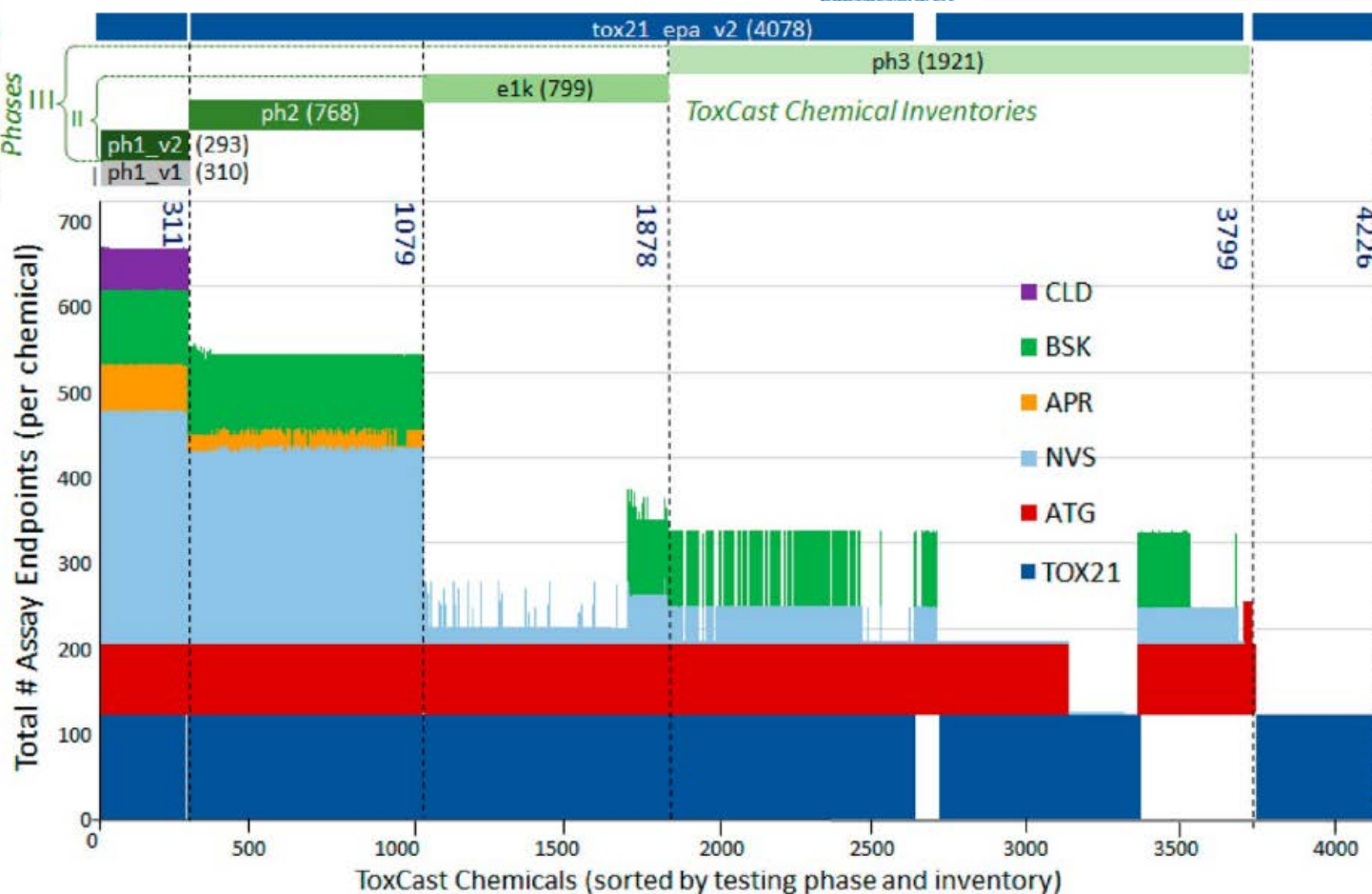
[pubs.acs.org/crt](https://pubs.acs.org/crt)

## Chemical Research in Toxicology

### ToxCast Chemical Toxicology

Ann M. Richard,<sup>\*,†</sup> Ri  
Inthirany Thillainadara  
John F. Wambaugh,<sup>†</sup>  
Antony J. Williams,<sup>†</sup> S

ToxCast Testing Phases



# Single Click to View Data

**EPA** United States Environmental Protection Agency

Home Advanced Search Batch Search Lists Predictions Downloads

Search All Data

Chemistry Dashboard | TOXCAST\_PHASEII

TOXCAST\_PhaseII - EPA ToxCast Screening Library (Phase II Subset)

Search TOXCAST\_PhaseII Chemicals

**List Details**

Description: TOXCAST\_PhaseII is the full set of 1864 chemicals screened in Phase II of the ToxCast screening program, consisting of the reprocurd Phase I chemical inventory (TOXCAST\_ph1v2), together with the TOXCAST\_ph2 and TOXCAST\_e1k sublists. At the time of the initial ToxCast Phase II public data release (Dec 2013), the e1k chemical subset had undergone limited screening in endocrine-related assays, whereas the ph1\_v2 and ph2 subsets (totaling 1061 chemicals) were more completely screened in both ToxCast Phase I assays and assays added in Phase II; all Phase II sublists were also included in Tox21 testing. For more details, see [TOXCAST](#)

Number of Chemicals: 1864

Download / Send  Sort by: DTXSID  1864 chemicals Hide:  Select all

Download as

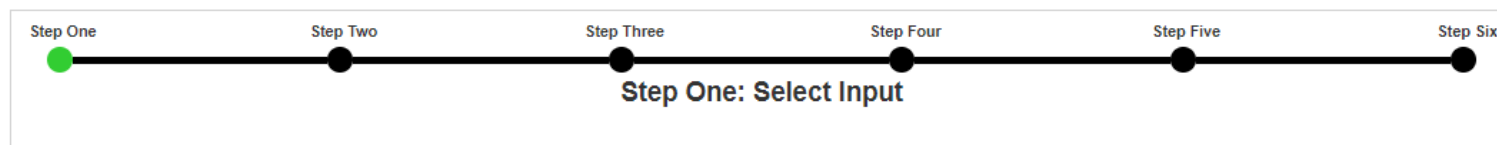
- TSV
- Excel
- SDF
- Send to
- Batch search

**Chemical Cards:**

- Amitrole**  
61-82-5  
Nc1ncnc
- Sodium L-ascorbate**  
134-03-2  
OC(O)[C@H](O)[C@@H](O)O[Na+]
- Aspartame**  
22839-47-0  
CC(=O)N[C@@H](Cc1ccccc1)C(=O)N[C@@H](C)C(=O)O
- Benzyl acetate**  
140-11-4  
CC(=O)OCc1ccccc1

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

# Batch Searching for Data for Thousands of Chemicals



Please enter one identifier per line

#### Select Input Type(s)

- ☐ Chemical Name
- ☐ CASRN
- ☐ InChIKey ☐ Skeleton
- ☐ DSSTox Substance ID
- ☐ MS-Ready Formula(e) ?
- ☐ Exact Formula(e)
- ☐ Monoisotopic Mass

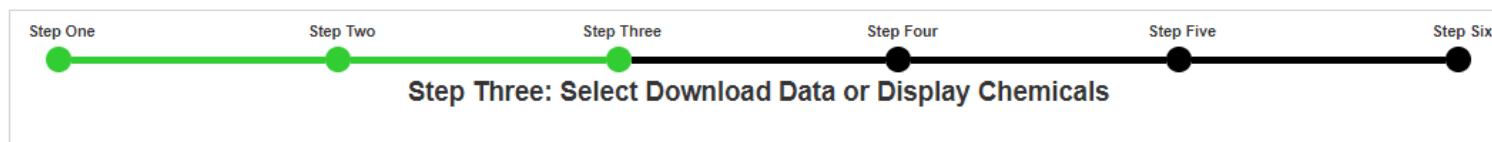
Enter Identifiers to Search (searches should be limited to <1000 identifiers)



A large, empty rectangular text input area with a light gray background and a vertical scrollbar on the right side.

Display All Chemicals

Downl



Please enter one identifier per line

#### Select Input Type(s)

- ☐ Chemical Name
- ☒ CASRN
- ☐ InChIKey ☐ Skeleton
- ☐ DSSTox Substance ID
- ☐ MS-Ready Formula(e) ?
- ☐ Exact Formula(e)
- ☐ Monoisotopic Mass

Enter Identifiers to Search (searches should be limited to <1000 identifiers)

30567-87-4  
2444-90-8  
67013-64-3  
551-04-2  
183614-42-8  
78238-97-8  
828254-85-9  
62411-64-7  
67223-12-5  
87923-90-8

Display All Chemicals

Download Chemical Data

# Batch Search

## Select Output Format

Excel ▼

## Customize Results

- ☐ Select All
- ☐ Select All In Lists

## Chemical Identifiers

- ☒ DTXSID ⓘ
- ☒ Chemical Name ⓘ
- ☐ CAS-RN ⓘ
- ☐ InChIKey ⓘ
- ☐ IUPAC Name ⓘ
- ☐ Synonyms and Identifiers ⓘ

## Structures

- ☐ Mol File ⓘ
- ☐ SMILES ⓘ
- ☐ InChI String ⓘ
- ☐ MS-Ready SMILES ⓘ
- ☐ QSAR-Ready SMILES ⓘ

## Intrinsic And Predicted Properties

- ☐ Molecular Formula ⓘ
- ☐ Average Mass ⓘ
- ☐ Monoisotopic Mass ⓘ
- ☐ OPERA Model Predictions ⓘ
- ☐ TEST Model Predictions ⓘ

## Metadata

- ☐ Curation Level Details ⓘ
- ☐ Data Sources ⓘ Details ⓘ
- ☐ Assay Hit Count ⓘ
- ☐ Include links to Active Assays ⓘ
- ☐ NHANES/Predicted Active Assays ⓘ
- ☐ Include ToxVal Data Availability ⓘ
- ☐ Number of PubMed Articles ⓘ
- ☐ Abstract Sifter Input File (Beta) ⓘ
- ☐ MetFrag Input File(Beta) ⓘ
- ☐ IRIS ⓘ
- ☐ PPRTV ⓘ
- ☐ PubChem Data Sources ⓘ
- ☐ ToxPrint fingerprints ⓘ
- ☐ CPDat Product Occurrence Count ⓘ

Checking this Assay Hit Count box inserts the number of assays that the chemical is tested in as well as the percent of assays for which the chemical is active.



# Downloadable Results

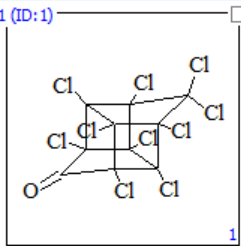
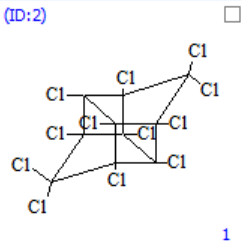
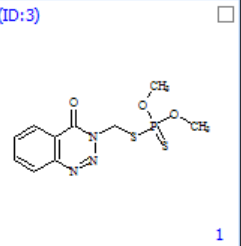
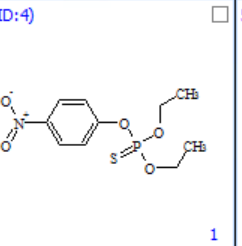
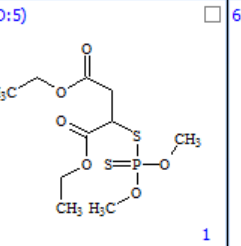
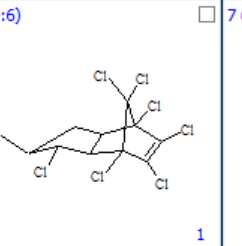
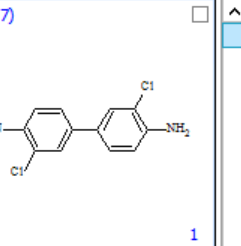
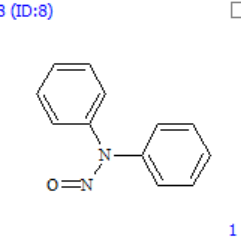
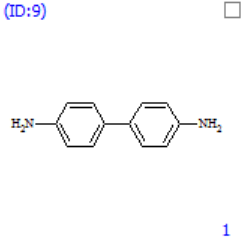
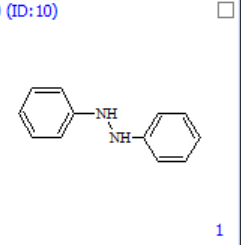
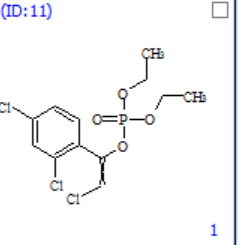
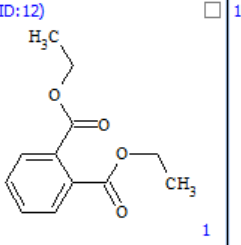
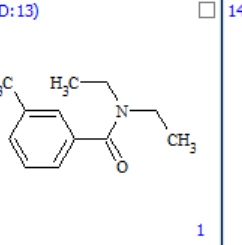
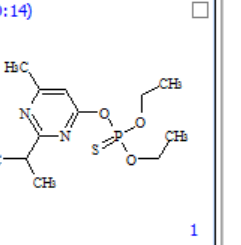
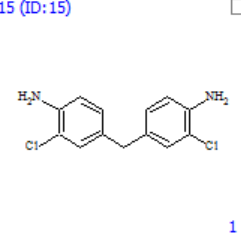
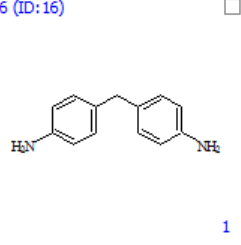
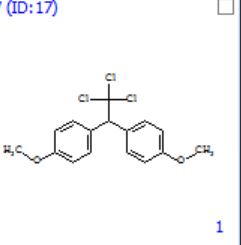
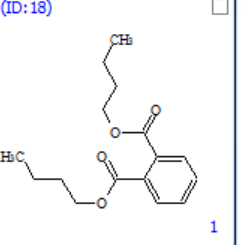
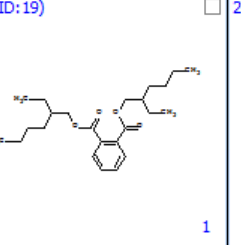
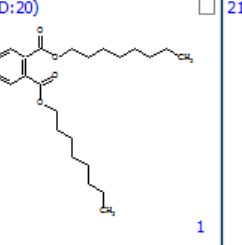
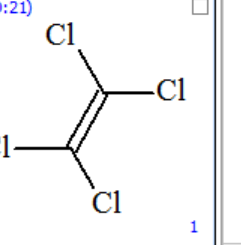
|   | A         | B                     | C         | D        | E                            | F        | G        | H      | I        | J           | K                      | L       | M       | N    | O     |
|---|-----------|-----------------------|-----------|----------|------------------------------|----------|----------|--------|----------|-------------|------------------------|---------|---------|------|-------|
|   | DTXSID    | PREFERRED_NAME        | CASRN     | INCHIKEY | SMILES                       | EXPOCAST | EXPOCAST | HNANES | DATA_SOL | TOXVAL_DATA | TOXCAST_PERCENT_ACTIVE | TOXCAST | PUBCHEM | IRIS | PPRTV |
| 1   | DTXSID002 | 1,2-Dichloropropane   | 78-87-5   | KNKRKFAL | CC(CI)CCI                    | 3.34e-06 | Y        | -      | 100      | Y           | 0.0                    | 0/113   | 89      | Y    | Y     |
| 2   | DTXSID002 | 2,4-Dinitrophenol     | 51-28-5   | UFBJCMHN | OC1=C(C(=O)C=C1)[N+](=O)[O-] | 6.19e-08 | Y        | -      | 111      | Y           | 6.3                    | 32/508  | 154     | Y    | Y     |
| 3   | DTXSID002 | Ethylene oxide        | 75-21-8   | IAYPIBMA | S C1CO1                      | -        | -        | -      | 85       | Y           | -                      | -       | 144     | -    | -     |
| 4   | DTXSID002 | Dichloromethane       | 75-09-2   | YMMVLUFA | CICCI                        | 0.02e-06 | Y        | -      | 110      | Y           | 0.88                   | 1/113   | -       | Y    | -     |
| <b>PREFERRED_NAME CASRN TOXVAL_DATA TOXCAST_%_ACTIVE TOXCAST_NUMBER PUBCHEM_DATA_S IRIS PPRTV</b> |           |                       |           |          |                              |          |          |        |          |             |                        |         |         |      |       |
| 1   |           | 1,2-Dichloropropane   | 78-87-5   | Y        |                              |          | 0.0      |        |          | 0/113       |                        |         | 89      | Y    | Y     |
| 2   |           | 2,4-Dinitrophenol     | 51-28-5   | Y        |                              |          | 6.3      |        |          | 32/508      |                        |         | 154     | Y    | Y     |
| 3   |           | Ethylene oxide        | 75-21-8   | Y        |                              |          | -        |        |          | -           |                        |         | 144     | -    | -     |
| 4   |           | Dichloromethane       | 75-09-2   | Y        |                              |          | 0.88     |        |          | 1/113       | -                      |         | -       | Y    | -     |
| 5   |           | 1,2-Propylene glycol  | 57-55-6   | Y        |                              |          | 2.04     |        |          | 11/539      |                        |         | 472     | Y    | Y     |
| 6   |           | 1,1,1-Trichloroethane | 71-55-6   | Y        |                              |          | 0.0      |        |          | 0/113       |                        |         | 86      | Y    | -     |
| 7   |           | Trichloroethylene     | 79-01-6   | Y        |                              |          | 3.54     |        |          | 4/113       |                        |         | 124     | Y    | -     |
| 8   |           | Chloromethane         | 74-87-3   | Y        |                              |          | -        |        |          | -           |                        |         | 64      | Y    | Y     |
| 9   |           | n-Hexane              | 110-54-3  | Y        |                              |          | 0.0      |        |          | 0/113       |                        |         | 1027    | Y    | Y     |
| 10  |           | Disulfoton            | 298-04-4  | Y        |                              |          | 7.15     |        |          | 48/671      |                        |         | 93      | Y    | Y     |
| 22  | DTXSID102 | Chlorine              | 7782-50-5 | KZBUYRJD | CICI                         | -        | -        | -      | 58       | Y           | -                      | -       | 39      | Y    | -     |
| 23  | DTXSID102 | Chloroethane          | 75-00-3   | HRYZWHH  | CCCCI                        | -        | -        | -      | 71       | Y           | -                      | -       | 75      | Y    | Y     |
| 24  | DTXSID102 | Chloroform            | 67-66-3   | HEDRZPFG | CIC(CI)CI                    | 3.5e-06  | Y        | -      | 110      | Y           | 0.0                    | 0/113   | 170     | Y    | -     |
| 25  | DTXSID102 | 1,1-Dichloroethane    | 75-34-3   | SCYULBFZ | CC(CI)CI                     | 1.2e-08  | Y        | -      | 93       | Y           | 2.65                   | 3/113   | 194     | Y    | Y     |
| 26  | DTXSID102 | Endosulfan            | 115-29-7  | RDYMFUSU | CIC1=C(CI)C=C1               | 1.36e-07 | Y        | -      | 101      | Y           | 22.8                   | 153/671 | 98      | Y    | Y     |
| 27  | DTXSID102 | Kepone                | 143-50-0  | LHHGDZSE | CIC12C(=O)C1                 | 1.94e-07 | Y        | -      | 84       | Y           | 36.42                  | 216/593 | 57      | Y    | -     |

Worksheet1

# SDF Download

ACD/Spectrus DB: Database Window - [C:\USERS\AW...OWNLOADS\CHEMISTRYDASHBOARD-ADVANCEDSEARCH\_2017-08-14\_12-14-55.SDF]

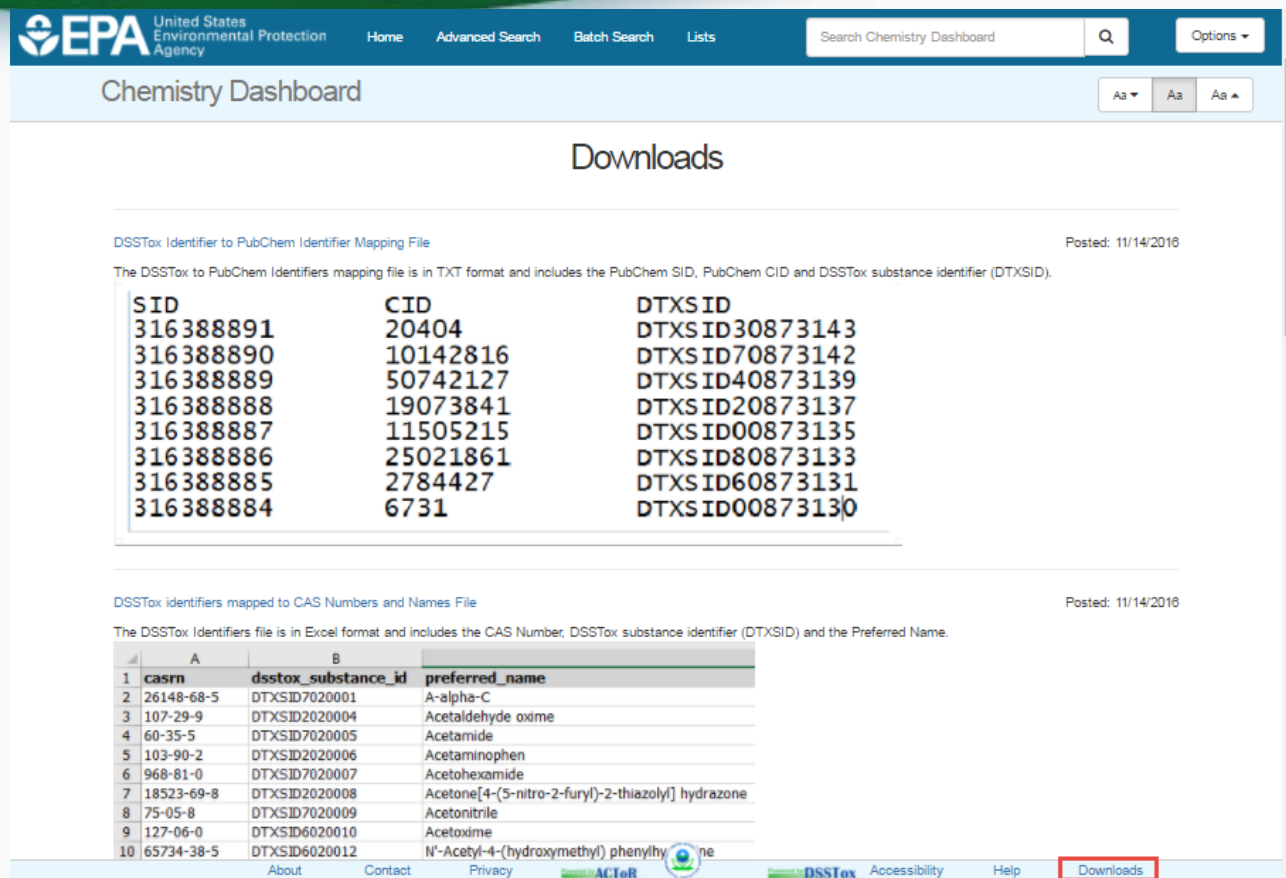
Database View Record Search Lists Plates Options ACD/Labs Help

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

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

1-ChemSketch 2-Database 3-Processor

# Delivering our Chemistry Data



The screenshot shows the EPA Chemistry Dashboard with a 'Downloads' section. It features two download links for DSSTox data files, each with a table of sample data.

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

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

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

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

The footer of the dashboard includes links for About, Contact, Privacy, ACToR, DSSTox, Accessibility, Help, and Downloads (highlighted with a red box).

- Various types of data at FTP download site:  
[ftp://newftp.epa.gov/COMPTOX/Sustainable\\_Chemistry\\_Data/Chemistry\\_Dashboard](ftp://newftp.epa.gov/COMPTOX/Sustainable_Chemistry_Data/Chemistry_Dashboard)

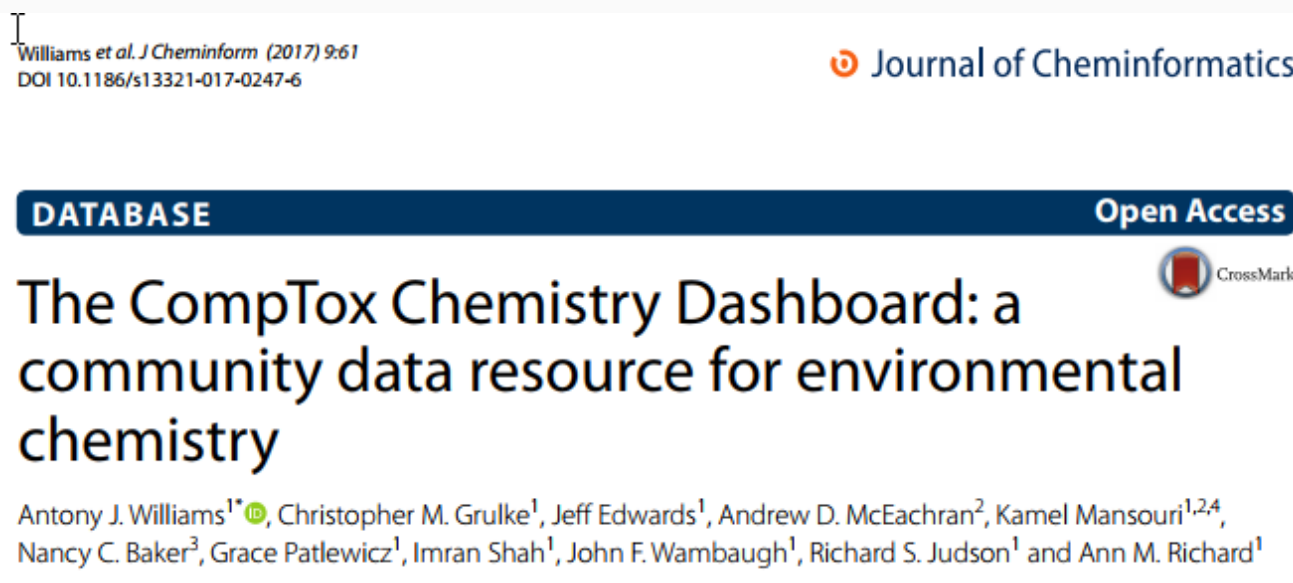
- The CompTox Chemistry Dashboard provides access to data for ~760,000 chemicals
- High quality data from ongoing curation efforts
- An integration hub for multiple “modules”
  - Experimental and predicted properties
  - Human and Ecological Hazard data
  - Exposure data – products, data in the environment
  - *In vitro* bioassay data – ToxCast/Tox21
  - Literature searching – Google Scholar and PubMed
  - Specialized searches – mass/formula for analytical support
  - Batch searching and Real Time Predictions
- The primary architecture for NCCT data

## Antony Williams

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[Williams.Antony@epa.gov](mailto:Williams.Antony@epa.gov)

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



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