Where are we now? Celebrating the 10th Incremental Release of the CompTox Chemicals Dashboard

Antony Williams

Center for Computational Toxicology and Exposure, U.S. Environmental Protection Agency, RTP, NC

The views expressed in this presentation are those of the author and do not necessarily reflect the views or policies of the U.S. EPA
• A Short History of the Dashboard
• What is the dashboard used for?
• New capabilities, data and lists
• Linkages – outbound and inbound
• Contributing to Data Quality
• Prototypes in progress
• What’s the Next Big Change?
THANK YOU TO ALL CONTRIBUTORS
Acknowledgments upfront...

- CCTE Members
  - CompTox Chemicals Dashboard Development Team
  - Principal Investigators and postdocs
  - Curation Team

- Collaborators across the agency for datasets, testing and cross-linking

- Contributors of datasets for registration

- And you, the users for support and feedback
A SHORT HISTORY of the DASHBOARD
Earlier Dashboard Applications

[Images of various dashboard applications, including a chemical structure of Bisphenol A and data visualization charts.]

EPA Dashboard Applications

EPA - ICBC ToxCast Dashboard

EDSP21 Dashboard
Retired Dashboards – Two Gone

- CompTox Chemicals Dashboard
- Aggregated Publicly Available Chemical Data
- ToxCast Dashboard
- EDSP21 Dashboard
- RapidTox
- Downloadable Data
ToxCast and EDSP21 Dashboards

- Both dashboards served valuable purposes for a number of years but blended in now

ANNOUNCEMENT

EDSP21 and ToxCast Dashboards have been Discontinued...

As of August 2019 the EDSP21 and ToxCast dashboards are no longer available. All functionality previously available in those dashboards has been migrated to the CompTox Chemicals Dashboard and new data has been made available. Specifically, the invitroDB database has been updated to version 3.2 (ftp://newftp.epa.gov/comptox/High_Throughput_Screening_Data/InVitroDB_V3.2/), a significant update including new chemicals and assays.

For further details about accessing the data and functionality from the older dashboards in the new CompTox Chemicals Dashboard reference the "CompTox Chemicals Dashboard Functionality" PDF and links below.
The CompTox Portal – get it here
https://comptox.epa.gov/
WHAT IS THE DASHBOARD USED FOR?
(and some what’s new)
CompTox Dashboard
Chemicals
DSSTox growth – 2007 to 2020
>7000 new chemicals added
CompTox Dashboard
Products and Use Categories

882 Thousand Chemicals

Chemical: Product/Use Categories
Assay/Gene

Search:
- hair color

- CPDat PRODUCT category: personal care hair color
  - hair colors and dyes characterized as permanent
- CPDat PRODUCT category: personal care hair color
  - hair colors and dyes characterized as for professional use
- CPDat PRODUCT category: personal care hair color
  - hair colors and dyes characterized as temporary
- CPDat PRODUCT category: personal care hair color
coloring products not otherwise categorized
- CPDat PRODUCT category: personal care hair color
  - chemical activators for hair coloring products
- CPDat PRODUCT category: personal care hair color developer
chemical developers for hair coloring products
- CPDat PRODUCT category: personal care hair color toner
color toners for hair coloring products
588k consumer products now in the database. Under constant curation and expansion...
Welcome to Factotum

Documents: 512,150
Products: 588,535
Extracted Chemicals: 3.9 million

Products Linked To PUCs: 67,206
Curated Chemical Records: 1.9 million
Unique DTXSIDs: 27,075
The Factotum Database

Formulation PUCs

<table>
<thead>
<tr>
<th>Category</th>
<th>Count</th>
</tr>
</thead>
<tbody>
<tr>
<td>Arts and crafts/Office supplies</td>
<td>3962</td>
</tr>
<tr>
<td>Cleaning products and household care</td>
<td>7917</td>
</tr>
<tr>
<td>Electronics/small appliances</td>
<td>2184</td>
</tr>
<tr>
<td>Home maintenance</td>
<td>5089</td>
</tr>
<tr>
<td>Landscape/Yard</td>
<td>1113</td>
</tr>
<tr>
<td>Personal care</td>
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<tr>
<td>Pesticides</td>
<td>1472</td>
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<tr>
<td>Pet care</td>
<td>1076</td>
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<tr>
<td>Sports equipment</td>
<td>139</td>
</tr>
<tr>
<td>Vehicle</td>
<td>1743</td>
</tr>
</tbody>
</table>
CompTox Dashboard
Assays and Genes

882 Thousand Chemicals

and curating data, major updates to the batch searching functionality and access to real time predictions for both physiochemical and toxicity endpoints. A list of release notes is available for your review. We look forward to your feedback.
Growth in *invitrodb* data 2015:2020
~150 new assay endpoints

- >140 assay endpoints and >700 chemicals added
- Data re-pipelined with new fitting procedures and ~200k new curve fits released with this version
- >140 endpoints annotated to genes

<table>
<thead>
<tr>
<th>Approx Year</th>
<th>Invitrodb Version (Public)</th>
<th># assay endpoints</th>
<th>#chemicals (total)</th>
<th>#curve fits (chemical-aeid pairs)</th>
<th>#assay endpoints annotated to gene</th>
<th>#unique target genes annotated</th>
</tr>
</thead>
<tbody>
<tr>
<td>2015</td>
<td>2.0</td>
<td>1192</td>
<td>9076</td>
<td>2,244,647</td>
<td>737</td>
<td>377</td>
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<tr>
<td>2018</td>
<td>3.1</td>
<td>1399</td>
<td>9214</td>
<td>3,281,340</td>
<td>1215</td>
<td>442</td>
</tr>
<tr>
<td>2019</td>
<td>3.2</td>
<td>1473</td>
<td>9224</td>
<td>3,525,844</td>
<td>1255</td>
<td>443</td>
</tr>
<tr>
<td>2020</td>
<td>3.3</td>
<td>1614</td>
<td>9949</td>
<td>3,720,594</td>
<td>1398</td>
<td>492</td>
</tr>
</tbody>
</table>
SOME EXAMPLES OF USAGE
Find me all “conazoles”
What chemicals in what use category?
“What’s in eye liner?”
Access *In Vitro* Bioactivity Data

ToxCast and Tox21
Access *In Vitro* Bioactivity Data

**ToxCast and Tox21**

![Bisphenol A](image)

**GC Data ID**

<table>
<thead>
<tr>
<th>Grade</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pass</td>
<td>Putty/60% and MN confirmed</td>
</tr>
</tbody>
</table>

**ToxCast/Tox21**

- A Single Assay Can Have Multiple Charts
- Representative Samples Only
- NCATS Summary

**Time series**

- A431ca (8 of 66 selected)
- Alltrans (26 of 165 selected)
- Bio Marc (9 of 174 selected)
- Nova serum (59 of 161 selected)
- NIEHS Lab (1 of 1 selected)
- CalixDirect (3 of 46 selected)
- ACEA Biomarkers (4 of 6 selected)
- NIEHS Lab (1 of 1 selected)
- Tox21/NCATS (69 of 247 selected)
- NCATS Simms Lab (8 of 26 selected)
- Targovy Lab (16 of 18 selected)
- Odyssey (11 of 17 selected)
- LifeTech/Expression Analysis (5 of 181 selected)
- Casest (2 of 24 selected)
- Sema Biomarker Discovery (5 of 11 selected)
- University of Pittsburgh Johnhro Lab (4 of 4 selected)

![Graphs](image)
GenRA (Generalised Read-Across)
Related Substances
e.g. Transformation Products

Aniline
62-53-3 | DTXSID8020090
Search by DSSTox Substance Id.
Related Substances for Markush

(C10-C16) Alkylbenzenesulfonic acid
68584-22-5 | DTXSID2028723
Searched by DSSTox Substance Id.

- **Searched Chemical**
  - (C10-C16) Alkylbenzenesulfonic acid
    - CASRN: 68584-22-5
    - DTXSID: DTXSID2028723
    - TOCAST: 56/235

- **Predecessor Component**
  - Alkylbenzenesulfonate, linear
    - CASRN: 92915-29-2
    - DTXSID: DTXSID3020041
    - TOCAST: 25

- **Component**
  - 4-(Dodecan-6-y)benzene-1-sulfonic acid
    - CASRN: 23003-92-1
    - DTXSID: DTXSID30869093
    - TOCAST: 1

- **Component**
  - 4-(Dodecan-4-y)benzene-1-sulfonic acid
    - CASRN: NOCAS, 863870
    - DTXSID: DTXSID40862870
    - TOCAST: 1

- **Component**
  - 4-(Dodecan-5-y)benzene-1-sulfonic acid
    - CASRN: NOCAS, 811097
    - DTXSID: DTXSID40861097
    - TOCAST: 1

- **Component**
  - 4-(Undecan-6-y)benzene-1-sulfonic acid
    - CASRN: NOCAS, 861146
    - DTXSID: DTXSID40861146
    - TOCAST: 1

- **Component**
  - 4-(Decan-4-y)benzenesulfonic acid
    - CASRN: NOCAS, 891333
    - DTXSID: DTXSID40891333
    - TOCAST: 1

- **Component**
  - 4-(Decan-5-y)benzenesulfonic acid
    - CASRN: NOCAS, 891564
    - DTXSID: DTXSID40891564
    - TOCAST: 1

- **Component**
  - 4-(Decan-6-y)benzenesulfonic acid
    - CASRN: NOCAS, 891689
    - DTXSID: DTXSID40891689
    - TOCAST: 1

- **Markush Child**
  - 4-Undecylbenzenesulfonic acid
    - CASRN: 121-65-3
    - DTXSID: DTXSID055643
    - TOCAST: 1
Identifiers to Support Searches

Bisphenol A
80-05-7 | DTXSID7020182
Searched by DSSTox Substance Id.

Synonym
- Bisphenol A
- 4,4’-(Propane-2,2-diyldiphenol
- Phenol, 4,4’-(1-methylene)bis-
- 80-05-7
- BPA
- 4,4’-(Propane-2,2-diyldiphenol
- Phenol, 4,4’-(1-methylene)bis-
- 4-06-00-06717
- (4,4’-Di(hydroxyphenyl)dimethylmethane
- 2,2-Bis(4-hydroxyphenyl)propane
- 2,2-Bis(4-hydroxyphenyl)propane
- 2,2-Bis(4-hydroxyphenyl)propane
- 2,2-Di(Hydroxyphenyl)Propane
- (De)alkylated Species
- 2,2-Bis(4-Hydroxyphenyl)Propane
- 2,2-Bis(4-Hydroxyphenyl)Propane
- 2,2-Bis(4-Hydroxyphenyl)Propane
- 2,2-Bis(4-Hydroxyphenyl)Propane
Abstract Sifter – PubMed Integration
searching >30 million abstracts

2,3,7,8-Tetrachlorodibenzo-p-dioxin
1746-01-6 | DTXSID2021315
Searched by Expert Validated Synonym.

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

1495 of 1495 articles loaded...

Optionally, edit the query before retrieving.

("1746-01-6 OR "2,3,7,8-Tetrachlorodibenzo-p-dioxin" OR "Tetrachlorodibenzo-dioxin") AND (cancer OR neoplasm OR carcinogen*)

To find articles quickly, enter terms to sift abstracts.

- dioxin
- cancer
- mortality

<table>
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<tr>
<th>dioxin</th>
<th>cancer</th>
<th>mortality</th>
<th>Total</th>
<th>PMID</th>
<th>Year</th>
<th>Title</th>
<th>Authors</th>
<th>Journal</th>
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<td>☑️</td>
<td>☑️</td>
<td>☑️</td>
<td>20</td>
<td>27897234</td>
<td>2015</td>
<td>Association between dioxin and cancer incidence and mortality.</td>
<td>Xu, Ye, Huang, Chen, Wu, Huang, Hu, Xia, Yi</td>
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<td>☑️</td>
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<td>16</td>
<td>9559713</td>
<td>1998</td>
<td>Estimation of the cumulative exposure to polychlorinated dibenzo-p-dioxins in residents of a residential area.</td>
<td>Fleisch-Jarjus, Steinford, Gier, Becher</td>
<td>Environmental health perspectives</td>
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</tbody>
</table>
Mass and Formula Searches
Supporting Mass Spectrometry
"MS-Ready" structures for non-targeted high-resolution mass spectrometry screening studies

Andrew D. McEachran, Kamel Mansouri, Chris Grulke, Emma L. Schymanski, Christoph Ruttkies and Antony J. Williams

Journal of Cheminformatics 2018 10:45
https://doi.org/10.1186/s13321-018-0299-2 © The Author(s) 2018
Received: 16 May 2018 | Accepted: 21 August 2018 | Published: 30 August 2018
MS-Ready Structures

**LEGEND:** Name, SMILES
DTXSID | InChIKey 1st Block
CAS | Monoiso. Mass | logP | Sources
Data on: Toxicity | Exposure | Bioassays

**Nicotine**
CN1CCC[C@H]1C1=CN=CC=C1
DTXSID1020930 | SNICXCGAKADSCV
54-11-5 | 162.1157 | 0.929 | 72
Tox: yes | Expo: yes | Bioassay: yes

**D-Nicotine**
CN1CC[C@H]1C1=CN=CC=C1
DTXSID004635 | SNICXCGAKADSCV
25162-00-9 | 162.1157 | 0.929 | 20
Tox: no | Expo: yes | Bioassay: yes

**Nicotine hydrochloride**
CI.CN1CCC[C@H]1C1=CN=CC=C1
DTXSID602093 | HDBTCAJIMNEXW
2820-51-1 | 198.0924 | 0.929 | 9
Tox: no | Expo: yes | Bioassay: yes

**Benzoic acid, 2-hydroxy-, compd. with 3-[(2S)-1-methyl-2-pyrrolidinyl]pyridine (1:1)**
OC(=O)C1=C(O)CC=C1.CN1CCC[C@H]1C1=CN=CC=C1
DTXSID5075319 | AIWPBPUA6MKNS
29790-52-1 | 300.1474 | 0.929 | 6
Tox: no | Expo: yes | Bioassay: no

**DL-Nicotine-d3**
[2H][2H][2H]N1CC1C1C1=CN=CC=C1
DTXSID92444666 | SNICXCGAKADSCV
165.1345 | 0.929 | 1
Tox: no | Expo: no | Bioassay: no
Find me all salts of...

Silver perfluorooctanoate
335-93-3 | DTXSID00880127
Searched by DSSTox Substance Id.
Real-Time Predictions
## Real-Time Predictions

<table>
<thead>
<tr>
<th>Property</th>
<th>Experimental Value</th>
<th>Consensus</th>
<th>Hierarchical clustering</th>
<th>Single model</th>
<th>Group contribution</th>
<th>Nearest neighbor</th>
</tr>
</thead>
<tbody>
<tr>
<td>96 hour fathead minnow LC50</td>
<td>5.000 -Log10(mol/L) 3.057 mg/L</td>
<td>5.194 -Log10(mol/L) 1.958 mg/L</td>
<td>5.692 -Log10(mol/L) 0.783 mg/L</td>
<td>5.151 -Log10(mol/L) 2.158 mg/L</td>
<td>4.064 -Log10(mol/L) 26.414 mg/L</td>
<td></td>
</tr>
<tr>
<td>48 hour D. magna LC50</td>
<td>4.827 -Log10(mol/L) 4.553 mg/L</td>
<td>4.920 -Log10(mol/L) 2.579 mg/L</td>
<td>5.266 -Log10(mol/L) 1.657 mg/L</td>
<td>5.317 -Log10(mol/L) 1.473 mg/L</td>
<td>3.805 -Log10(mol/L) 47.846 mg/L</td>
<td></td>
</tr>
<tr>
<td>48 hour T. pyriformis IC50</td>
<td>5.209 -Log10(mol/L) 1.892 mg/L</td>
<td>5.074 -Log10(mol/L) 2.501 mg/L</td>
<td>5.343 -Log10(mol/L) 1.387 mg/L</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Oral rat LD50</td>
<td>2.059 -Log10(mol/kg) 2669702 mg/kg</td>
<td>2.028 -Log10(mol/kg) 2889132 mg/kg</td>
<td>2.095 -Log10(mol/kg) 2494135 mg/kg</td>
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<td></td>
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<tr>
<td>Developmental toxicity</td>
<td>true</td>
<td>true</td>
<td>true</td>
<td></td>
<td></td>
<td></td>
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<tr>
<td>Ames mutagenicity</td>
<td>false</td>
<td>false</td>
<td>false</td>
<td></td>
<td></td>
<td></td>
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<td>Estrogen Receptor Binding</td>
<td>false</td>
<td>false</td>
<td>false</td>
<td>false</td>
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<tr>
<td>Normal boiling point</td>
<td>372.1 °C</td>
<td>331.0 °C</td>
<td>479.8 °C</td>
<td>305.5 °C</td>
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<td></td>
</tr>
<tr>
<td>Melting point</td>
<td>133.9 °C</td>
<td>126.4 °C</td>
<td>138.6 °C</td>
<td>136.7 °C</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Flash point</td>
<td>232.7 °C</td>
<td>282.4 °C</td>
<td>240.2 °C</td>
<td>175.7 °C</td>
<td></td>
<td></td>
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</table>
NEW CAPABILITIES, DATA AND LISTS
Watch for our news
https://comptox.epa.gov/dashboard/news_info

CompTox Chemicals Dashboard

882 Thousand Chemicals

Latest News

10th Release of the CompTox Chemicals Dashboard Now Live July 12th 2020

July 21st, 2020 at 9:32:02 PM

The 10th release of the Dashboard is now live with >7000 additional substances added to the dataset, updates to Bioactivity Data (ToxCast/Tox21), updates to the ToxVaI data (under the Hazard tab), a new Safety Tab integrating the Globally Harmonized System of Classification and Labeling of Chemicals (via PubChem), over thirty new lists and a number of bug fixes. Our next release is scheduled for late Spring/Early Summer 2021, and is presently in development. It will be a full re-architecting of the entire application. Watch this space for updates. The release addresses a number of minor bugs and includes a short list of additional functionality as described in the Release Notes here.
• A detailed list of new functionality and fixes

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<tr>
<th>New Functionality</th>
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<tr>
<td>ICD-4105</td>
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<td>ICD-4294</td>
</tr>
<tr>
<td>ICD-4147</td>
</tr>
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<td>ICD-4248</td>
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<td>ICD-4233</td>
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<td>ICD-4103</td>
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<td>ICD-4140</td>
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<td>ICD-4153</td>
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<td>ICD-4201</td>
</tr>
<tr>
<td>ICD-4017</td>
</tr>
<tr>
<td>ICD-4285</td>
</tr>
</tbody>
</table>
New Safety Tab
Integrating PubChem GHS Data

Atrazine
1912-24-9 | DTXSID9020112
Searched by DSSTox Substance Id.

GHS Data

CID 2256

Atrazine

GHS Classification

Showing 6 of 6

Pictogram(s)

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Signal

Warning

H317: May cause an allergic skin reaction [Warning Sensitization, Skin]

H373 **: Causes damage to organs through prolonged or repeated exposure [Warning Specific target organ toxicity, repeated exposure]

H400: Very toxic to aquatic life [Warning Hazardous to the aquatic environment, acute hazard]

H410: Very toxic to aquatic life with long lasting effects [Warning Hazardous to the aquatic environment, long-term hazard]

GHS Hazard Statements

Precautionary Statement Codes

(The corresponding statement to each P-code can be found at the GHS Classification page.)
Over 260 Lists Now Available

• Lists ranging from 3 to >62,200 chemicals
• 27 different PFAS lists – structures and non-structure lists
• Lists added to support specific programs
Disinfectant By-Products
82 to 619 chemicals

LIST: Disinfection By-products (Richardson et al)


Number of Chemicals: 619

619 chemicals

Benzene acid
CASRN:65-85-0
DTXSID:DTXSID020143
TOXCAST:12/837

Benzyl chloride
CASRN:100-44-7
DTXSID:DTXSID0020153
TOXCAST:12/3235

Bromochloromethane
CASRN:75-27-4
DTXSID:DTXSID1020198
TOXCAST:12/235

2-Bromo-1-ethanol
CASRN:540-51-2
DTXSID:DTXSID802000
TOXCAST:12/235
Consolidated List of Lists under EPCRA/CERCLA/CAA §112(r) (June 2019 Version)

List Details

Description: The List of Lists is a consolidated list of chemicals subject to the Emergency Planning and Community Right-to-Know Act (EPCRA), Comprehensive Environmental Response, Compensation, and Liability Act (CERCLA), and Section 112(r) of the Clean Air Act (CAA). This is a partial mapping and under constant curation.

Number of Chemicals: 1363

1363 chemicals

- Acetamide
  CASRN: 60-35-5
  DTXSID: DTXSID7020005
  TOXCAST: 17/664

- Acetonitrile
  CASRN: 75-05-8
  DTXSID: DTXSID7020009
  TOXCAST: 2/235

- Acrolein
  CASRN: 107-02-8
  DTXSID: DTXSID5020023
  TOXCAST: 2/233

- Acrylamide
  CASRN: 70-05-8
  DTXSID: DTXSID5020027
  TOXCAST: 22/887
Curated Wikipedia
>12,000 chemicals

List Details

Description: Wikipedia includes data for thousands of chemicals. ChemBoxes and DrugBoxes includes data such as CAS Registry Numbers, SMILES and InChis. This list is an assembly from various Wikipedia pages and is a list under ongoing curation and expansion.
Number of Chemicals: 12861

1250 of 12861 chemicals loaded

Select all  Download  Send to Batch Search  Default  CASRN  DTXSID  TOXCAS

Hide chemicals that are:
Filter by Name or CASRN
Wikipedia serves the “snippet”

Sarin (NATO designation GB [short for G-series, “G”]) is an extremely toxic synthetic organophosphorus compound. A colourless, odourless liquid, it is used as a chemical weapon due to its extreme potency as a nerve agent. Exposure is lethal even at very low concentrations, where death can occur within one-to-ten minutes after direct inhalation of a lethal dose, due to suffocation from lung muscle paralysis, unless antidotes are quickly administered.

Read more
Other Lists of Interest

- Storage Tanks – Above Ground/Underground
- IRIS Chemicals refreshed to >600 chemicals
- Azo dyes (decompose to aromatic amines)
- Curated CASMI (Critical Assessment of Small Molecule Identification) datasets
Lists provide a landscape overview

### Presence in Lists

**Federal**
- TOXCASTT Phase II - EPA ToxCast Screening Library (Phase II Subset)
- TOXCAST Phase II - EPA ToxCast Screening Library (Phase II Subset)
- TOXCAST_ph2 - EPA ToxCast Screening Library (ph2 Subset)
- CHEMINV: EPA Chemical Inventory for ToxCast
- TOXCAST: EPA ToxCast Screening Library
- ENDOCRINE: ESP Universe of Chemicals
- ECOTOX: Ecotoxicology knowledgebase
- WATER: EPA Chemicals in hydraulic fracturing fluids Table H-2
- WATER: EPA; Chemicals associated with hydraulic fracturing
- EPA: Consumer Products Suspect Screening Result
- TOXCAST: EPA ToxCast Screening Assay In Vitro DB Version 3
- EPA: High Production Volume List
- CHEMINV: ToxCast/Tox21 Chemical inventory available as DMSO solutions (20181123)
- TOX21SL: Tox21 Screening Library
- LIST: Substances Added to Food (formerly EAFUS)
- TSCA Active Inventory non-confidential portion (updated March 20th 2020).

**US State**
- None.

**International**
- Canadian Domestic Substances List 2019
- FOOD: EFSA OpenFoodTox
- NORMAN: KEMI List of Substances on the Market

**Other**
- COSMOS DB cosmetics database
- NORMAN: REACH Chemicals List Provided to NORMAN Network
- NORMAN: Norman Network Suspect Screening List (SUZDAT)
- EPA: CPDAT, Chemical and Products Database
- Global harmonization system aggregated chemical data list (skin and eyes)
- MASSPECDB: Thermo's mzCloud Database
- NORMAN: Combined 2000/2006 EU Cosmetic Ingredients Inventory
- WATER: STOFF-IDENT Database of Water-Relevant Substances
- ESTROGEN: Integrated pathway model for the Estrogen Receptor
- NEURO: DNT Screening Library
- PESTICIDES|EPA: Pesticide Chemical Search Database
- ARTICLE: Collaborative Estrogen Receptor Activity Prediction Project (COMPARA)
- LIST: Wikipedia chemicals
- LIST: Hazardous Substances Data Bank
- PESTICIDES|EPA: List of Inert Ingredients Food and Nonfood Use UPDATED 10/25/2019
• Batch search a list of chemicals to identify presence in >280 lists
Select lists of Interest & Export File

Batch Search

Step Four: Select Data Output Format and Choose Data Fields to Download

Enter Identifiers to Search (One per line. Searches should be limited to <5000 identifiers.)
- DTXSID1020069
- DTXSID6020123
- DTXSID2020183
- DTXSID7020186
- DTXSID3020001
- DTXSID9020324
- DTXSID5020491
- DTXSID6020511
- DTXSID6021082
- DTXSID1021118

Select Input Type(s)
- Identifiers
  - Chemical Name
  - CASRN
  - InChIKey
  - DSSTox Substance ID
  - DSSTox Compound ID
  - InChIKey Skeleton
  - MS-Ready Formula(e)
  - Exact Formula(e)
  - Monoisotopic Mass

Select Output Format:
- Excel

Download

Presence in Lists:
- 30CFR115.4 Designation of Hazardous Substances (Above Ground Storage Tanks)
- ACHR1555 Extremely Hazardous Substance List and Threshold Planning Quantities
- ACHR1575 Acute Exposure Guideline Levels
- ANDROGEN Androgen Receptor Chemicals
- ADELS Acute Exposure Guideline Levels
## Cross-walking lists of interest

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LINKAGES
OUTBOUND and INBOUND
Increasingly important identifier

The DTXSID

Atrazine
1912-24-9 DTXSID9020112

[Chemical structure of Atrazine]

Wikipedia

Atrazine is a herbicide of the triazine class. It is used to prevent pre-emergence broadleaf weeds in crops such as maize (corn) and sugarcane and on turf such as golf courses and residential lawns. Atrazine’s primary manufacturer is Syngenta and it is one of the most widely used herbicides in US and Australian agriculture.

As of 2001, atrazine was the most commonly detected pesticide contaminating drinking water in the United States. Studies suggest it is an endocrine disruptor.

Read more

Quality Control Notes

Intrinsic Properties

- Molecular Formula: C_{9}H_{14}ClN_{3}
- Average Mass: 215.69 g/mol
- Monoisotopic Mass: 215.093773 g/mol

Structural Identifiers

- IUPAC Name: 6-Chloro-N-2-ethyl-N-4-(propan-2-yl)-1,3,5-triazine-2,4-diamine
- SMILES: CCN1=NC(NC(C)Cl)=NC(Cl)=N1

Find All Chemicals

Isotope Mass Distribution
In-links from various sources

- Wikipedia
- AOP Wiki
- PubChem
- MassBank
- UniChem
The DTXSID Identifier

Wikidata:Property proposal/DTXSID

DSSTOX substance identifier [ edit ]

Originally proposed at Wikidata:Property proposal/Natural science

- **Done:** DSSTox substance ID (P3117) (Talk and documentation)

**Description**
The DTXSID is the DSSTox substance identifier used in the Environmental Protection Agency CompTox Dashboard.

**Data type**
External identifier

**Domain**
chemical substance (Q75529)

**Example**
benzene (Q2270) → DTXSID3039242

**Planned use**
Adding DTXSIDs to @wikidata using a bot or possible Mix&Match, based on InChiKey matches and this CCZero data on Figshare:
https://figshare.com/articles/Mapping_file_of_InChiStrings_InChiKeys_and_DTXSIDs_for_the_EPA_CompTox_Dashboard/3578313/1

**Formatter URL**
https://comptox.epa.gov/dashboard/$1

**Motivation**
The Environmental Protection Agency (G16919823)'s CompTox Dashboard is a fairly new website, but the DSSTox project exists for much longer (Distributed structure-searchable toxicity (DSSTox) public database network: a proposal (G26701365)). The Dashboard aggregates over 720 thousand chemical substances and is open data. The CompTox dashboard also provides access to synonyms, experimental and predicted property data, product and functional use details and EPA's Toxcast Bioassay data. The DTXSIDs are unique substance identifiers, already been included into PubChem and the EBI Unichem InChiKey mapping files. The DTXSIDs will also be included into the BridgeDb metabolite mapping databases on short notice. Egon Willighagen [talk] 17:48, 24 August 2016 (UTC)
Increasing number of outlinks

- External Links reduce time to discovery
# State-Specific Water Quality Standards Effective under the Clean Water Act (CWA)

EPA has compiled state, territorial, and authorized tribal water quality standards that EPA has approved or are otherwise in effect for Clean Water Act purposes. This compilation is continuously updated as EPA approves new or revised WQPs.

In instances when state-specific water quality standards have not been developed or approved by EPA, the Agency will propose and/or promulgate standards for a state until such time as the state submits and EPA approves their own standards. Any federally-proposed or promulgated replacement water quality standards are also identified.

Please note the water quality standards may contain additional provisions outside the scope of the Clean Water Act, its implementing federal regulations, or EPA’s authority. In some cases, these additional provisions have been included as supplementary information.

EPA is posting the water quality standards as a convenience to users and has made a reasonable effort to assure their accuracy. Additionally, EPA has made a reasonable effort to identify parts of the standards that are approved, disapproved, or are otherwise not in effect for Clean Water Act purposes.

- See EPA’s ComTox Chemical Dashboard for more information on this chemical.

<table>
<thead>
<tr>
<th>State</th>
<th>Parameter (the name used by the state)</th>
<th>Application</th>
<th>Criteria Magnitude</th>
</tr>
</thead>
<tbody>
<tr>
<td>Alaska</td>
<td>atrazine</td>
<td>drinking water MCL (water supply</td>
<td>drinking, culinary and food processing; contact recreation) (Human Health)</td>
</tr>
<tr>
<td>Arizona</td>
<td>atrazine</td>
<td>Domestic Water Source (DWS) (Human Health)</td>
<td>3 μg/l</td>
</tr>
<tr>
<td>Arizona</td>
<td>atrazine</td>
<td>Full-Body Contact (FBC) (Human Health)</td>
<td>32667 μg/l</td>
</tr>
<tr>
<td>Arizona</td>
<td>atrazine</td>
<td>Partial-Body Contact (PBC) (Human Health)</td>
<td>32667 μg/l</td>
</tr>
<tr>
<td>California Region 1 - North Coast</td>
<td>atrazine</td>
<td>municipal or domestic supply (Human Health)</td>
<td>0.0030 mg/l</td>
</tr>
<tr>
<td>California Region 2 - San Francisco Bay</td>
<td>atrazine</td>
<td>municipal supply</td>
<td>0.0030 mg/l</td>
</tr>
<tr>
<td>California Region 2 - Central Coast</td>
<td>atrazine</td>
<td>domestic or municipal supply</td>
<td>0.0030 mg/l</td>
</tr>
<tr>
<td>California Region 4 - Los Angeles</td>
<td>atrazine</td>
<td>municipal and domestic water supply (Human Health)</td>
<td>0.001 mg/l</td>
</tr>
<tr>
<td>California Region 9 - San Diego</td>
<td>atrazine</td>
<td>municipal or domestic supply (Human Health)</td>
<td>0.0030 mg/l</td>
</tr>
<tr>
<td>Colorado</td>
<td>atrazine</td>
<td>drinking water supply (Human Health)</td>
<td>3 μg/l</td>
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</table>
New Outlinks of Interest
PubChem Chemical Vendors

<table>
<thead>
<tr>
<th>Vendor</th>
<th>PubChem SID</th>
<th>Purchasable Chemical</th>
</tr>
</thead>
<tbody>
<tr>
<td>Yuhao Chemical</td>
<td>355047054</td>
<td>LT4922</td>
</tr>
<tr>
<td></td>
<td>347737622</td>
<td>LT6957</td>
</tr>
<tr>
<td>Achemo Scientific Limited</td>
<td>252453703</td>
<td>AC-11427</td>
</tr>
<tr>
<td>Sigma-Aldrich</td>
<td>329753681</td>
<td>31212_SI</td>
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<td></td>
<td>329756651</td>
<td>45330_SIGMA</td>
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<td></td>
<td>24871790</td>
<td>48187_SUPELCO</td>
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<tr>
<td></td>
<td>24872608</td>
<td>49085_SUPELCO</td>
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<tr>
<td></td>
<td>329769969</td>
<td>90935_SI</td>
</tr>
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<td></td>
<td>329823655</td>
<td>PS380-250MG_SUPELCO</td>
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<tr>
<td></td>
<td>24899206</td>
<td>PS380_SUPELCO</td>
</tr>
<tr>
<td>ZINC</td>
<td>256808431</td>
<td>ZINC3078958</td>
</tr>
<tr>
<td>Acadechem</td>
<td>321908354</td>
<td>ACDS-021206</td>
</tr>
</tbody>
</table>
New Outlinks of Interest
California EPA OEHHA

Atrazine

CAS Number
1912-24-9

Synonym(s)
Aatrex; Akticon; Argezin; Atranex; Atrataf; Atrazin; Atred; Atrex; Candex; Chromozin; Cyazin; Farmaco atrazine; Fenamine; Gesaprim; Inakor; Caswell No. 063; Oleogesaprim; Pitezin; Primatol; Primaze; Radazin; Strazine; Vectal; Weedex A; Wonuk; Zeapos; Zeazin; Zeazine; EPA Pesticide Code: 080803
CONTRIBUTING to DATA QUALITY
Ongoing Data Review
Thanks to our curators!

Cumulative Manual

Data Curation Level

- View the level of curation for any chemical
- If you see any issues let us know

**Record Information**

**Citation:** U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. https://comptox.epa.gov/dashboard/DTXSID3031864 (accessed July 23, 2020), Perfluorooctanesulfonic acid

**Data Quality:**

- **Level 1:** Expert curated, highest confidence in accuracy and consistency of unique chemical identifiers
- **Level 2:** Expert curated, unique chemical identifiers using multiple sources
- **Level 3:** Programmatically curated from high quality EPA source, unique chemical identifiers have no conflicts in ChemID and PubChem
- **Level 4:** Programmatically curated from ChemID, unique chemical identifiers have no conflicts in PubChem
- **Level 5:** Programmatically curated from ACToR or PubChem, unique chemical identifiers with low confidence, single public source
As users, please contribute

- We welcome your comments: [https://comptox.epa.gov/dashboard/contact_us](https://comptox.epa.gov/dashboard/contact_us)
Please help curate the data…

• Users can identify issues with all of our data
  – Suggest chemicals to add to lists
  – Suggest related substances – e.g. metabolites, degradants
  – Flag errors in the data – e.g. properties

• We are now receiving daily feedback – “Submit Comment”
Submit Comments
We will provide feedback...

New Comment

Details to be submitted with your comment

Text selected: Danish_EPA_SCPFAS_Report_2015
Found On: July 22nd 2020, 8:25:09 pm
Original Query: /dsstoxdb/results?search=PFOS#properties
Browser: Chrome 84

Comment

There appears to be a value missing associated with the "Danish_EPA_SCPFAS_Report_2015". Maybe worth checking if there should be a value added?

Email address

williams.antony@epa.gov

I'm not a robot

Submit
### Crowdsource Comments

<table>
<thead>
<tr>
<th>Chemical</th>
<th>Structure</th>
<th>Date</th>
<th>Comment</th>
<th>Resolution</th>
</tr>
</thead>
<tbody>
<tr>
<td>Oxazole, 2-ethyl-4,5-dimethyl-</td>
<td><img src="image1.png" alt="Structure" /></td>
<td>2020-07-22</td>
<td>4,5-Dimethyl-2-ethylxoxazole is just a BAD name - remove? Add 2-Ethyl-4,5-dimethylxoxazole WLN is T5N COJ B2 D1 E1 REAXYS/BRN is S07360 FEMA 3672 MFCD0036664 Barrie</td>
<td>Resolved</td>
</tr>
<tr>
<td>4-Decenoic acid, ethyl ester, (4E)-</td>
<td><img src="image2.png" alt="Structure" /></td>
<td>2020-07-22</td>
<td>Add names Ethyl (4E)-4-decenoate (uninverted CAS name) Ethyl (E)-dec-4-enoate (IUPAC) FEMA 3642 REAXYS/BRN 1770966 WLN 6U3YO2 &amp;&amp;E or trans Form REACH 278-509-4 (ex EINECS) PubChem CID 5362583 MFCD00015574 UNII-3189X5937N Barrie</td>
<td>Resolved</td>
</tr>
<tr>
<td>Hexanedioic acid, diisonyonyl ester</td>
<td><img src="image3.png" alt="Structure" /></td>
<td>2020-07-21</td>
<td>the tox cast curves for some chemicals will not display, specifically the toxcast/tox21 tab is missing from the left side menu on the dashboard. You can only display the toxcast summary (that shows that there are results from toxcast/tox21) or the toxcast models. Examples are 33703-08-1 and 27178-16-1.</td>
<td>Resolved</td>
</tr>
<tr>
<td>2-Pentenal, 5-(methylthio)-2-[(methylthio)methyl]-</td>
<td><img src="image4.png" alt="Structure" /></td>
<td>2020-07-20</td>
<td>2,8-Dithianon-4-en-4-carboxaldehyde should be aldehyde 2-Methyithiomethyl-5-methylthiopent-2-enal BAD name - remove, on corrected as below 5-(Methylthio)-2-(methylthio)methylpent-2-en-1-al 5-(Methylthio)-2-(methylthio)methylpent-2-enal known trivially as Methiolol REAXYS/BRN is 2241044 WLN is 1S3UYYH1S1 Barrie</td>
<td>Resolved</td>
</tr>
<tr>
<td>Dipentyl 2-hydroxybutanedioate</td>
<td><img src="image5.png" alt="Structure" /></td>
<td>2020-07-20</td>
<td>well known as Dipentyl malate WLN SOVQ1VOS Barrie</td>
<td>Resolved</td>
</tr>
<tr>
<td>Tricyclo[1.1.0.0^2,4^]tetraphosphane</td>
<td><img src="image6.png" alt="Structure" /></td>
<td>2020-07-20</td>
<td>This comment or question is asked of me somewhat frequently, is DTXSID1024382 white phosphorus as it is listed a synonym, or is it more appropriate to say DTXSID90923991 is white phosphorus? Any clarification that could be provided on DTXSID90923991’s entry on the Dashboard would be appreciated.</td>
<td>Resolved</td>
</tr>
</tbody>
</table>
PROTOTYPES in PROGRESS
Proof-of-Concept: Structure/Substructure/Similarity Searches
Other Prototypes in Progress

• “Structure Standardization” services to produce MS-Ready and QSAR-ready data
• Single predictions already available. Batch predictions in development.
“RapidTox” Proof-of-Concept
RapidTox Dashboard

Decision-support tool to integrate chemistry, toxicity and exposure information

Under different federal statutes, EPA makes a broad range of decisions to protect public health and the environment from unintended consequences of using chemicals. Decisions about chemicals are also made by other Federal Agencies, State Environmental and Health Agencies, International Governmental Agencies and Industry. As examples, there are specific federal laws for pesticides, drinking water contaminants, commercial and industrial chemicals, chemicals found on contaminated sites and endocrine disrupting chemicals.

These laws give EPA the authority to gather health, safety and exposure data on chemicals, require necessary testing, and control human and environmental exposures. EPA’s computational toxicology researchers are integrating available chemical information including chemistry, toxicity and exposure information into an online tool called RapidTox to help decision-makers quickly and efficiently evaluate chemicals. To help decision-makers leverage this information effectively, researchers are now customizing this tool to help EPA and states meet the requirements under various federal statutes as well as state and local laws.
An automated framework for compiling and integrating chemical hazard data

Leora Vegosen¹,² · Todd M. Martin²

Received: 3 October 2019 / Accepted: 13 December 2019 / Published online: 21 January 2020
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Now: “Hazard Comparison Dashboard”

- Watch this space....
WHAT’S THE NEXT BIG CHANGE?
• After 5 years & 10 releases, we have reached the end of this technology architecture
• The dashboard: a prototype that kept growing
• We are starting afresh with a new architecture based on a datahub and new user experience
• First release scheduled for March 2021
  – migration of existing capabilities
  – supporting increased frequency of data releases
  – existing dashboard will remain online for smooth transition
Short Term Goals for Release

• Using new table widgets to unify tabulated data handling across the application
• Rebuilding visualization widgets to support multiple applications
• Service-based architecture will ultimately provide **public API** to access datahub
• Faster, more flexible searching
Future Integration Planned…
The ACToR Database
The early days of the dashboard
https://jcheminf.springeropen.com/articles/10.1186/s13321-017-0247-6

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

Antony J. Williams¹*, Christopher M. Grulke¹, Jeff Edwards¹, Andrew D. McEachran², Kamel Mansouri¹,²,⁴, Nancy C. Baker³, Grace Patlewicz¹, Imran Shah¹, John F. Wambaugh¹, Richard S. Judson¹ and Ann M. Richard¹
We owe a great debt to the curators who have invested efforts over ~20 years
Downloadable Data Will Be Updated

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).

<table>
<thead>
<tr>
<th>SID</th>
<th>CID</th>
<th>DTXSID</th>
</tr>
</thead>
<tbody>
<tr>
<td>316388891</td>
<td>20404</td>
<td>DTXSID30873143</td>
</tr>
<tr>
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<td>10142816</td>
<td>DTXSID70873142</td>
</tr>
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<td>316388889</td>
<td>50742127</td>
<td>DTXSID40873139</td>
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<td>316388888</td>
<td>19073841</td>
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<td>25021861</td>
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<td>316388885</td>
<td>2784427</td>
<td>DTXSID0873131</td>
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<tr>
<td>316388884</td>
<td>6731</td>
<td>DTXSID00873130</td>
</tr>
</tbody>
</table>

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.

<table>
<thead>
<tr>
<th>casrn</th>
<th>dsstox_substance_id</th>
<th>preferred_name</th>
</tr>
</thead>
<tbody>
<tr>
<td>26148-68-5</td>
<td>DTXSID7020001</td>
<td>Acetaldehyde oxime</td>
</tr>
<tr>
<td>107-29-9</td>
<td>DTXSID200084</td>
<td>Acetamide</td>
</tr>
<tr>
<td>60-35-5</td>
<td>DTXSID200003</td>
<td>Acetaminophen</td>
</tr>
<tr>
<td>101-99-2</td>
<td>DTXSID200006</td>
<td>Acetaminophen</td>
</tr>
<tr>
<td>90-81-0</td>
<td>DTXSID200007</td>
<td>Acetoxycoumarin</td>
</tr>
<tr>
<td>18523-69-8</td>
<td>DTXSID200008</td>
<td>Acetone(4-(5-nitro-2-furyl)-2-thiazolyl) hydrazine</td>
</tr>
<tr>
<td>75-05-8</td>
<td>DTXSID200000</td>
<td>Acetone</td>
</tr>
<tr>
<td>127-96-0</td>
<td>DTXSID6020010</td>
<td>Acetone</td>
</tr>
</tbody>
</table>
Conclusion

• The Dashboard is our primary web-based tool for delivering data to the community
• Data growth continues unabated – new chemicals, toxicity data, products, predictions, \textit{in vitro} data…
• Data curation is a \textbf{critical} aspect of the project
• Proof-of-concept applications in development
  – Structure standardization (MS-Ready/QSAR-Ready)
  – Structure-substructure-similarity searching
  – Hazard Comparison Dashboard and RapidTox workflows
• Next release (March 2021) will be a full \textit{rebuild} of the architecture. Public API in development
Antony Williams
US EPA Office of Research and Development
National Center for Computational Toxicology (NCCT)
Williams.Antony@epa.gov
ORCID: https://orcid.org/0000-0002-2668-4821

(Please note I am one small cog in the engine that makes the dashboard happen…)