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EPA United States Environmental Protection Agency

# An Introduction and Demo of the CompTox Chemicals Dashboard

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**University of Copenhagen – November 2nd 2021**

# Recommended Reading

EPA United States Environmental Protection Agency

ELSEVIER

Environment International

Volume 154, September 2021, 106566


Review article

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

Antony J. Williams [a], Jason C. Lambert [a], Kris Thayer [b], Jean-Lou C.M. Dorne [c]

# The Charge for the Dashboard

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

# CompTox Chemicals Dashboard

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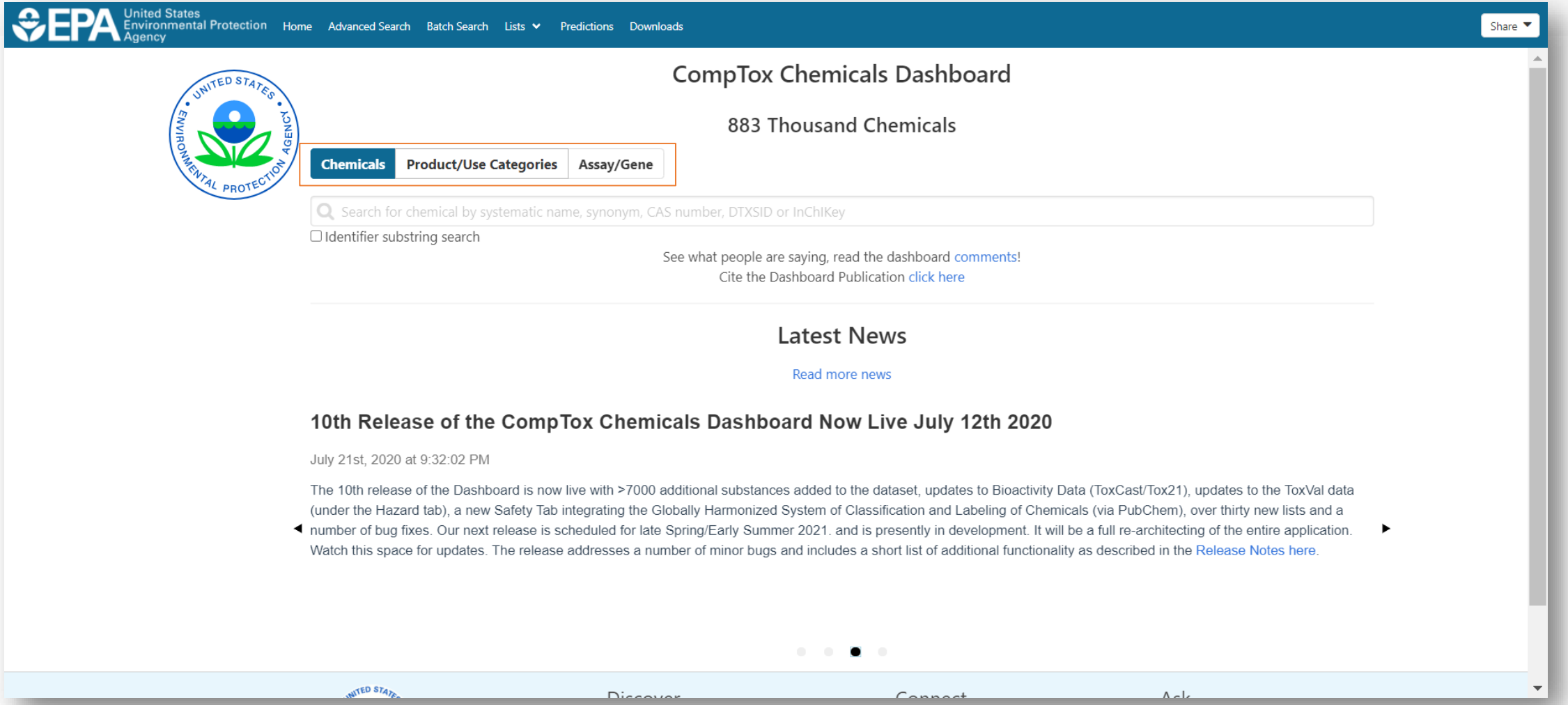
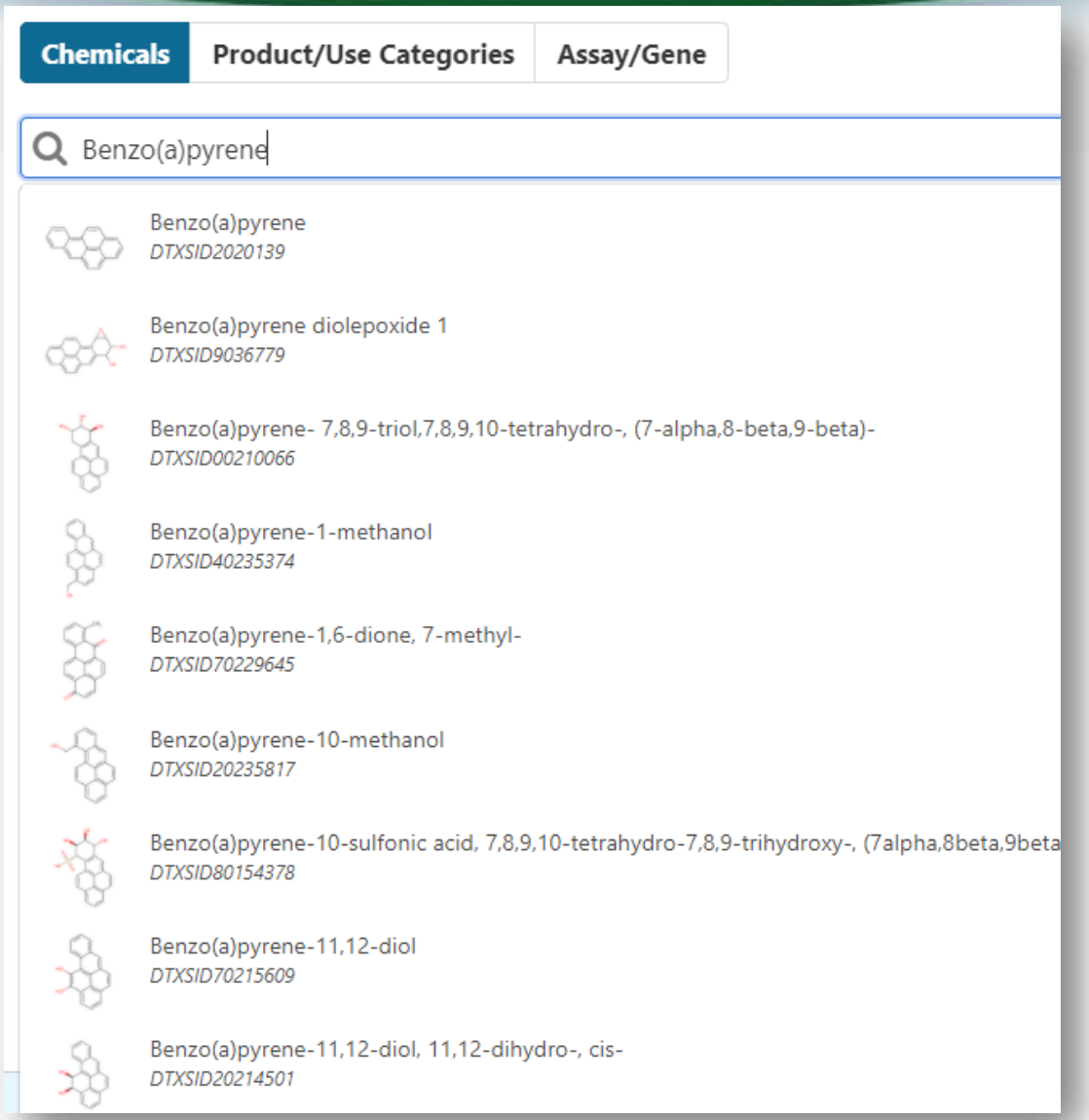
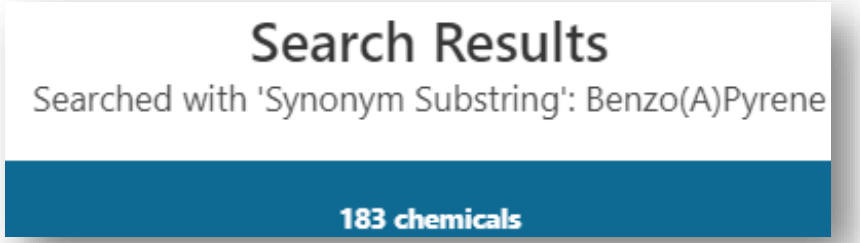
## 883k Chemical Substances



# BASIC Search

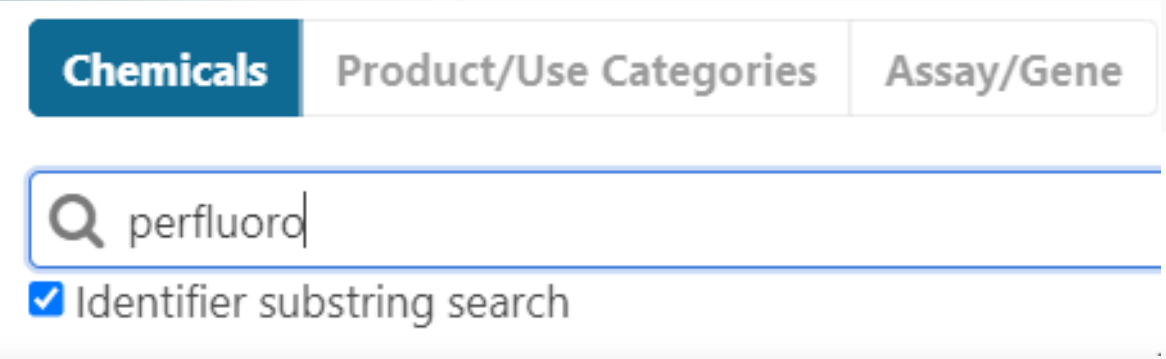


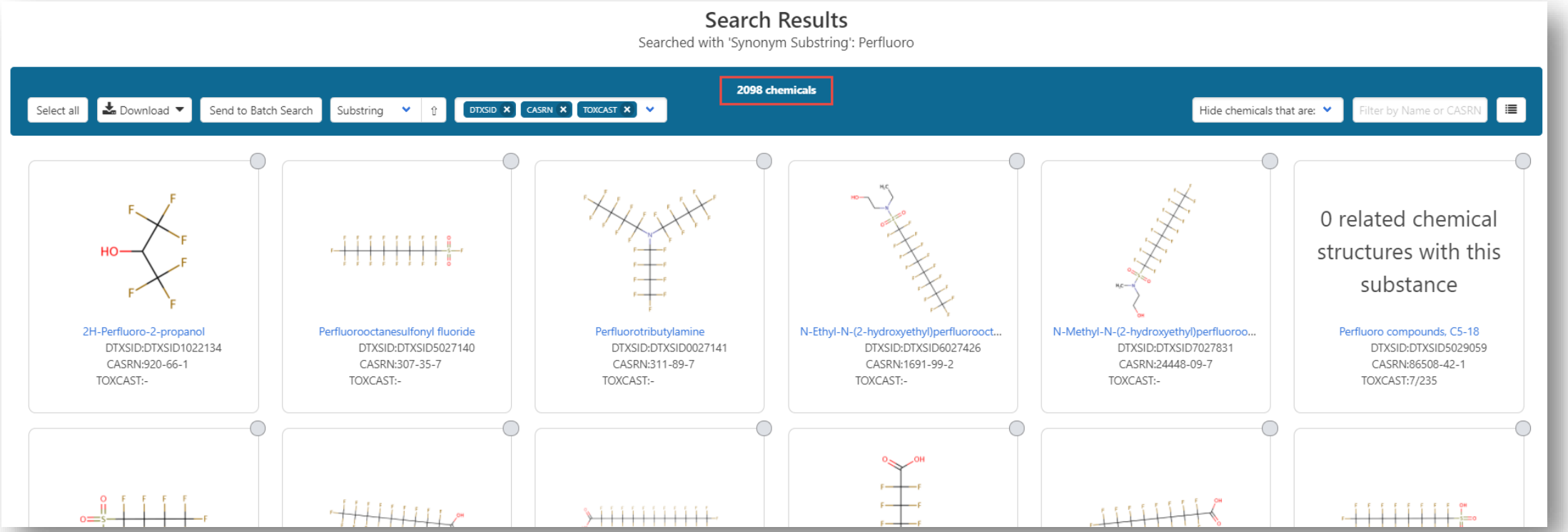

- Type ahead search using Names, synonyms and CASRNs
- Millions of identifiers
- Substring search



# Search for classes of chemicals

- Examples: “perfluoro”

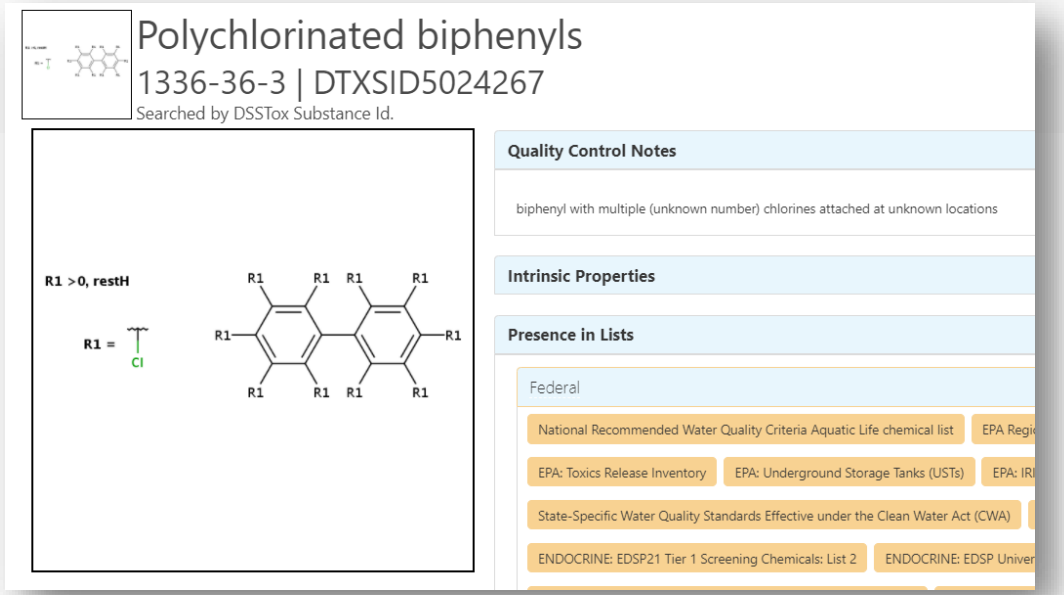


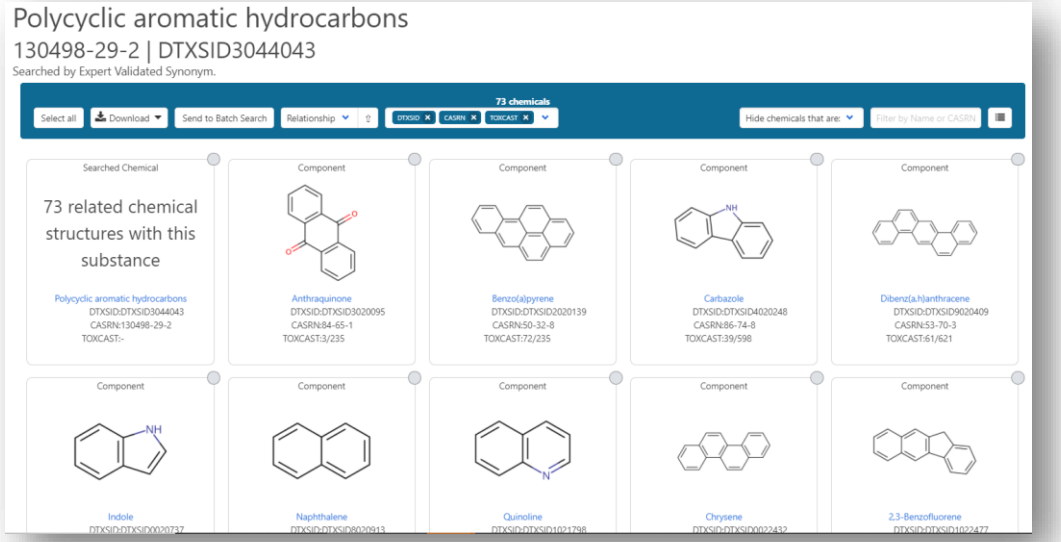
# Search for classes of chemicals

Examples:

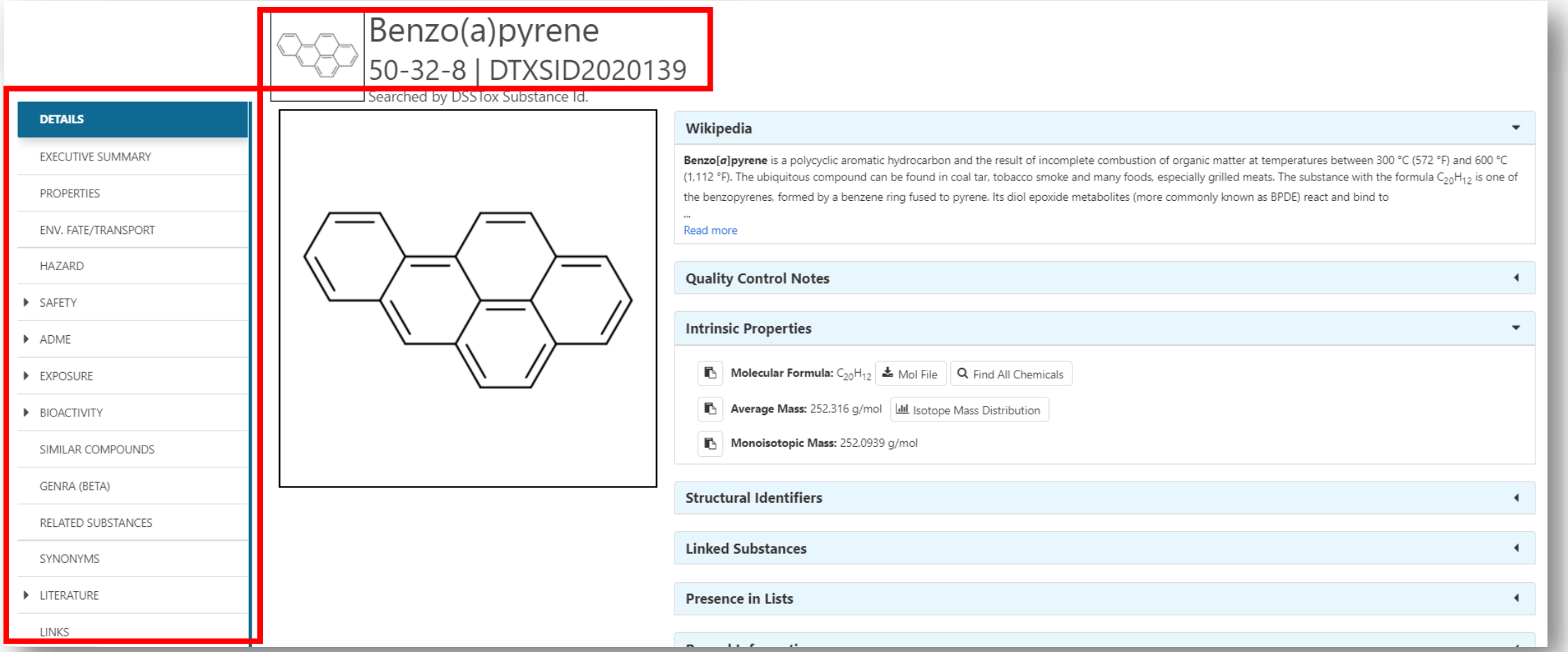
- PCBs (or polychlorinated biphenyls)




- Polycyclic aromatic hydrocarbons

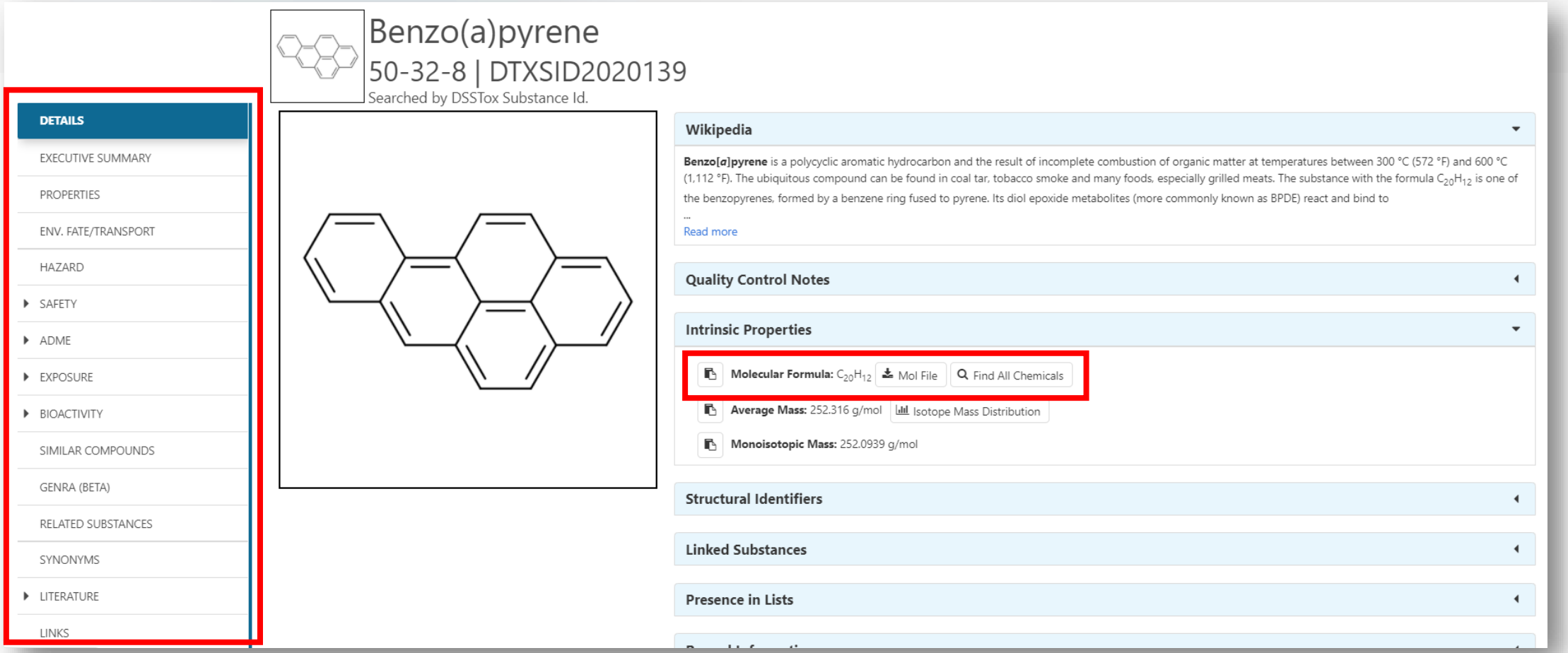


# Detailed Chemical Pages
# One more identifier – the DTXSID




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

# Detailed Chemical Pages
# Easy Navigation




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

# From the Chemical Details Page… all chemicals with same FORMULA

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**Intrinsic Properties**

**Molecular Formula:** $C_{20}H_{12}$ | Mol File | Find All Chemicals

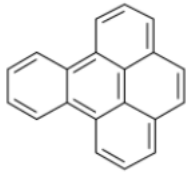
## Search Results

Searched by Exact Molecular Formula: C20H12.

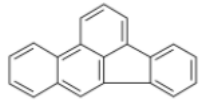
27 chemicals

Download | Send to Batch Search | Default | CASRN | DTXSID | Hide chemicals that are: | Filter by Name or C

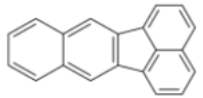
Benzo(a)pyrene
CASRN:50-32-8
DTXSID:DTXSID2020139



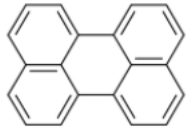
Benzo(e)pyrene
CASRN:192-97-2
DTXSID:DTXSID3023764



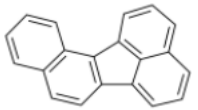
Benzo(b)fluoranthene
CASRN:205-99-2
DTXSID:DTXSID0023907



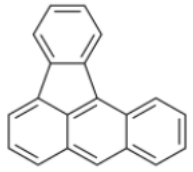
Benzo(k)fluoranthene
CASRN:207-08-9
DTXSID:DTXSID0023909



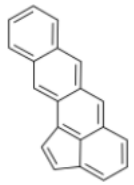
Perylene
CASRN:198-55-0
DTXSID:DTXSID4047753



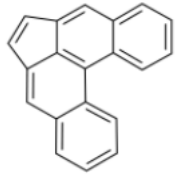
Benzo(j)fluoranthene
CASRN:205-82-3
DTXSID:DTXSID8052691



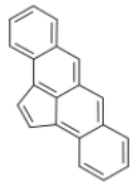
Benzo[a]fluoranthene
CASRN:203-33-8
DTXSID:DTXSID4059756



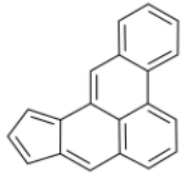
Cyclopenta(de)naphthacene
CASRN:16683-64-0
DTXSID:DTXSID80168197



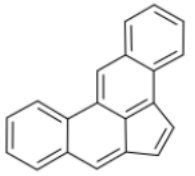
Benz(a)acephenanthrylene
CASRN:192-28-9
DTXSID:DTXSID70172748



Cyclopenta(fg)naphthacene
CASRN:19770-52-6
DTXSID:DTXSID40173469



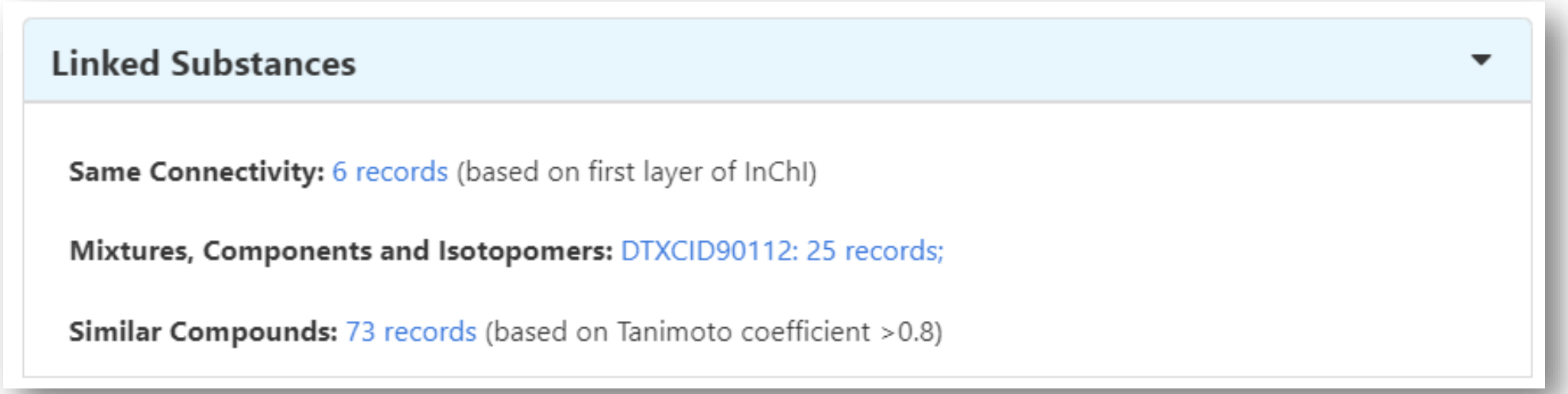
Benzo(de)cyclopent(a)anthracene
CASRN:198-46-9
DTXSID:DTXSID60173507



Benz(e)aceanthrylene
CASRN:199-54-2
DTXSID:DTXSID30173675

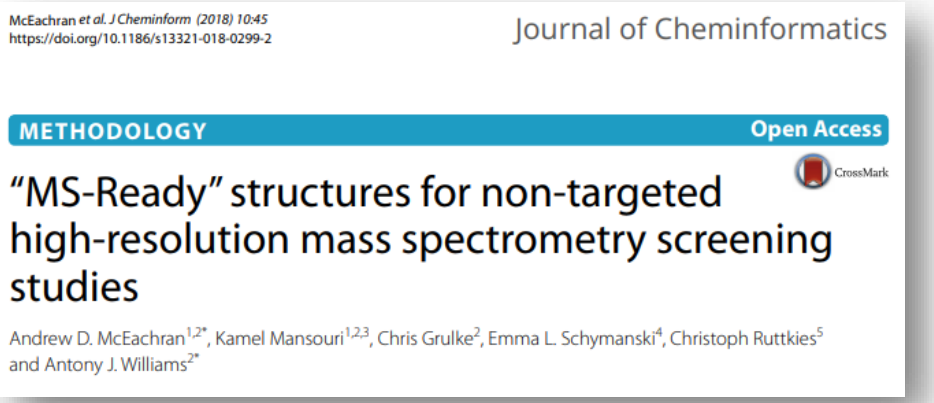
# How many chemicals are associated through LINKED SUBSTANCES?

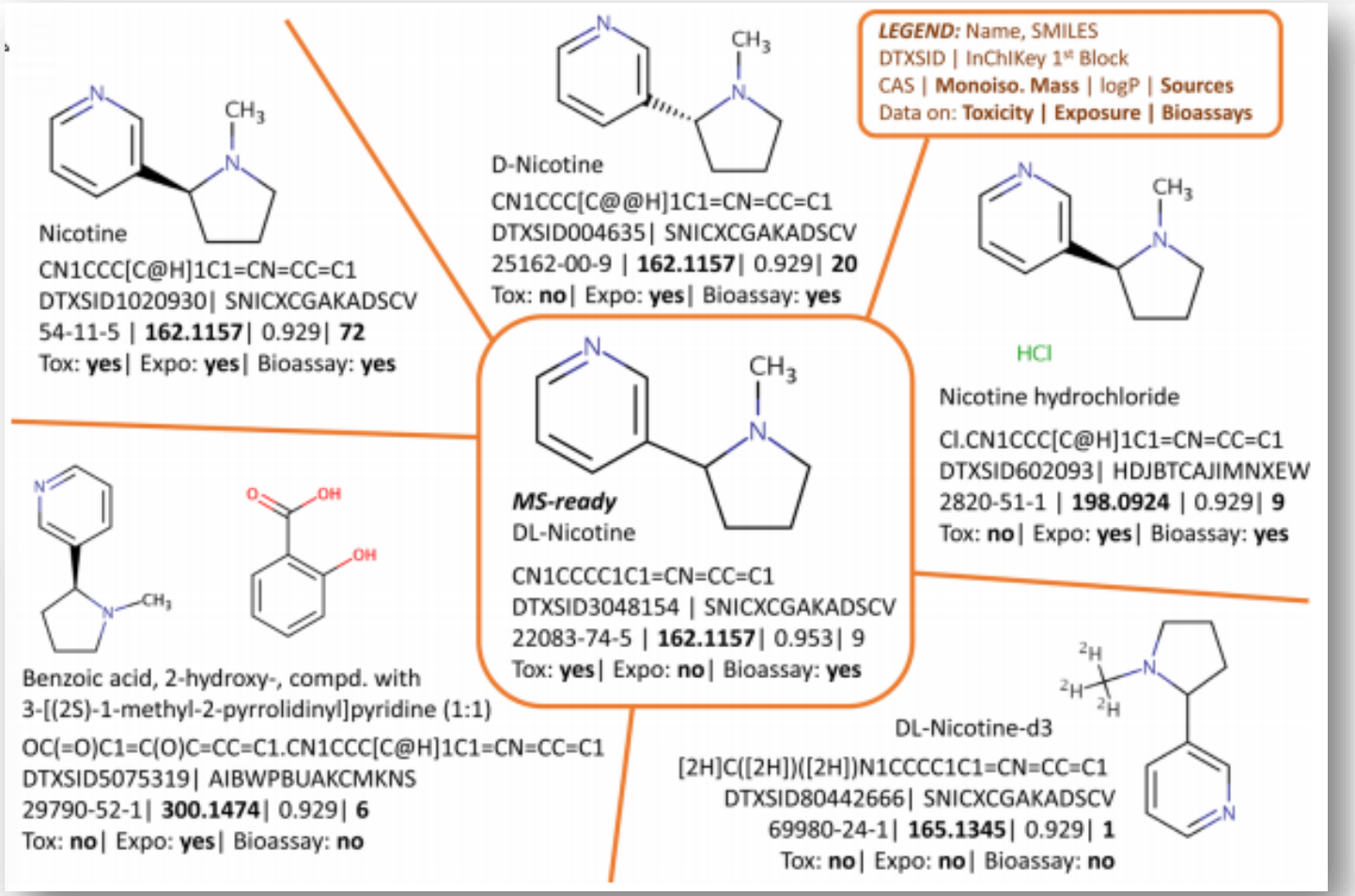
- Atrazine, is a herbicide – in MANY commercial products
- The dashboard has salt forms, isotopically labelled forms, multicomponent forms
- How do we identify what they are???



# Linked Substances – more interesting

- We map chemicals together using cheminformatics approaches
- Use desalting, destereo, split multicomponents etc to map chemicals together



# Atrazine Linked Substances

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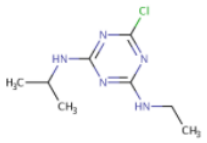
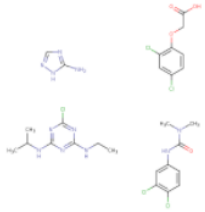
## MS-Ready Mappings of Atrazine (Isotopes pre-filtered)

20 of 25 chemicals visible

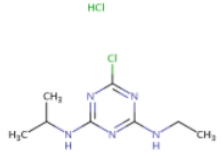
Select all | Download | Send to Batch Search | Default | DTXSID | CASRN | TOXCAST | Isotopes | Filter by Name or CASRN



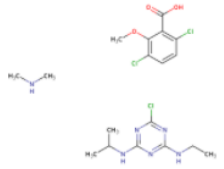
Atrazine
DTXSID:DTXSID9020112
CASRN:1912-24-9
TOXCAST:62/1024



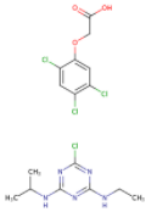
Anox M
DTXSID:DTXSID50156021
CASRN:128996-76-9
TOXCAST:-



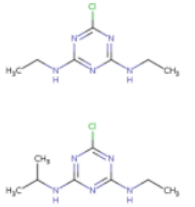
s-Triazine, 2-chloro-4-(ethylamino)-6-(is...
DTXSID:DTXSID30165459
CASRN:15386-47-7
TOXCAST:-



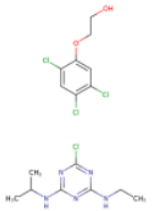
Marksman
DTXSID:DTXSID80166936
CASRN:160544-50-3
TOXCAST:-



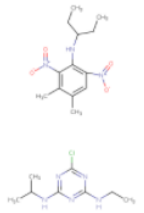
Acetic acid, (2,4,5-trichlorophenoxy)-, mi...
DTXSID:DTXSID70192527
CASRN:39283-62-0
TOXCAST:-



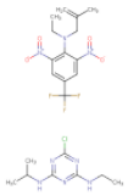
1,3,5-Triazine-2,4-diamine, 6-chloro-N,N...
DTXSID:DTXSID60192556
CASRN:39331-45-8
TOXCAST:-



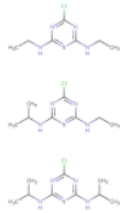
Buvinol
DTXSID:DTXSID10199555
CASRN:51602-05-2
TOXCAST:-



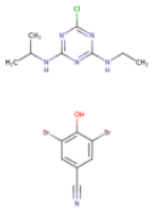
Atrazine mixture with pendimethalin
DTXSID:DTXSID10209527
CASRN:60704-01-0
TOXCAST:-



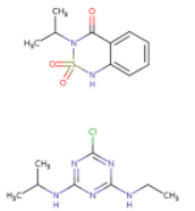
Maizor
DTXSID:DTXSID20215154
CASRN:64867-15-8
TOXCAST:-



Polytriazine
DTXSID:DTXSID00222508
CASRN:72172-70-4
TOXCAST:-

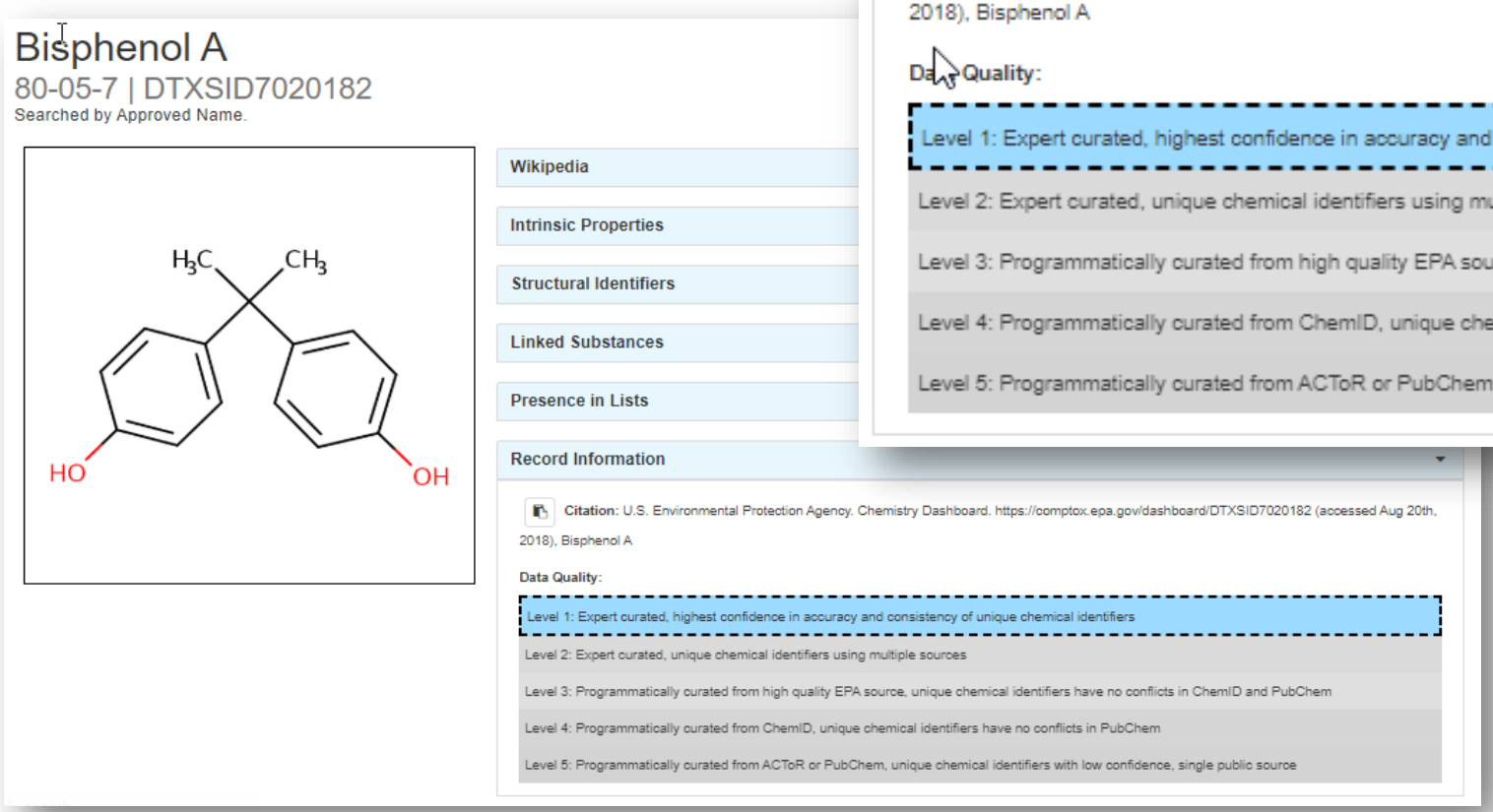


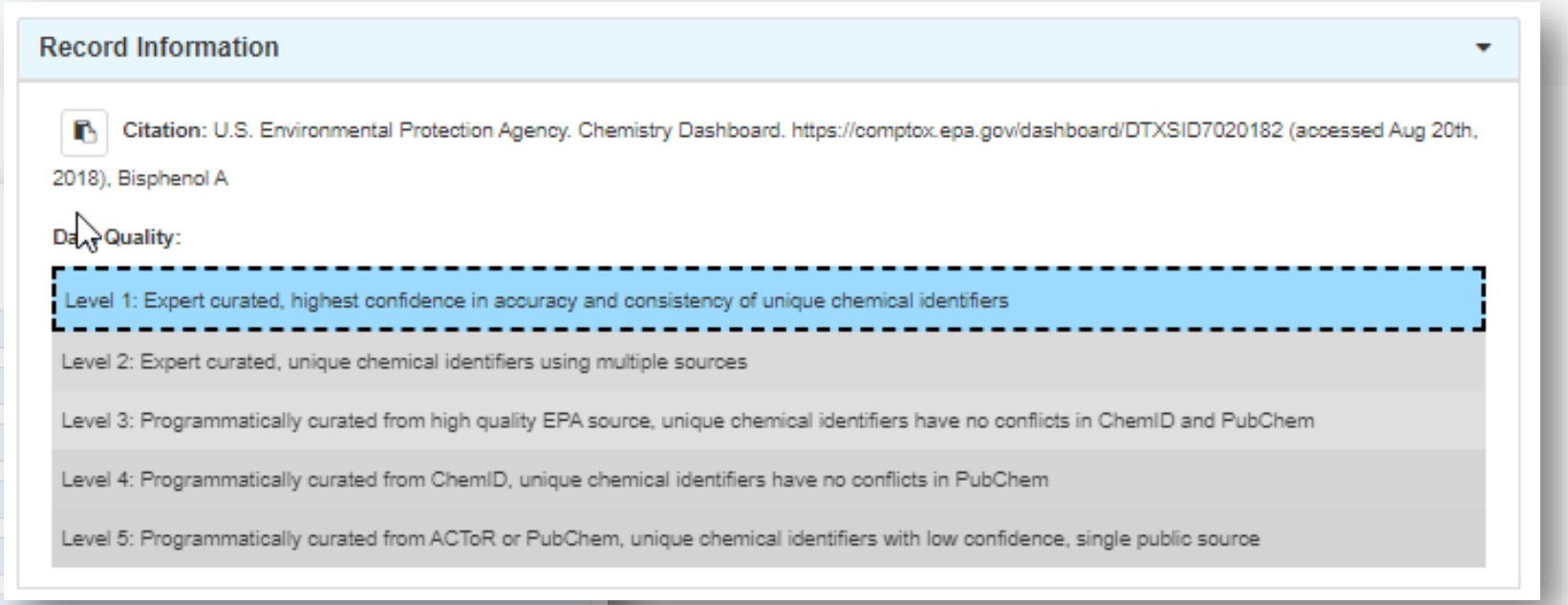
Benzonitrile, 3,5-dibromo-4-hydroxy-, m...
DTXSID:DTXSID20226063
CASRN:75084-56-9
TOXCAST:-



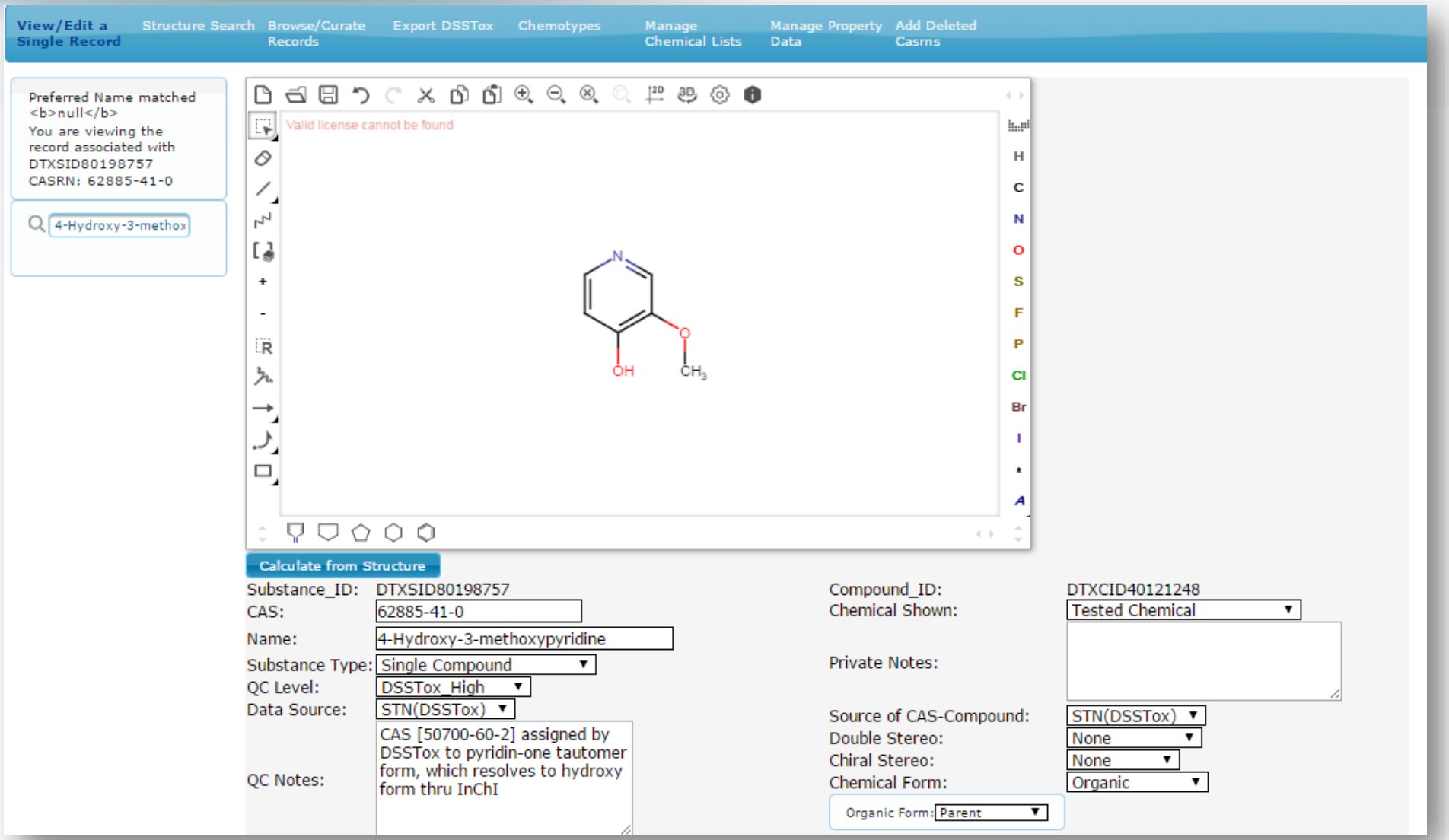
Bentazon / atrazine
DTXSID:DTXSID80226064
CASRN:75084-57-0
TOXCAST:-

# Record Information Quality Flags

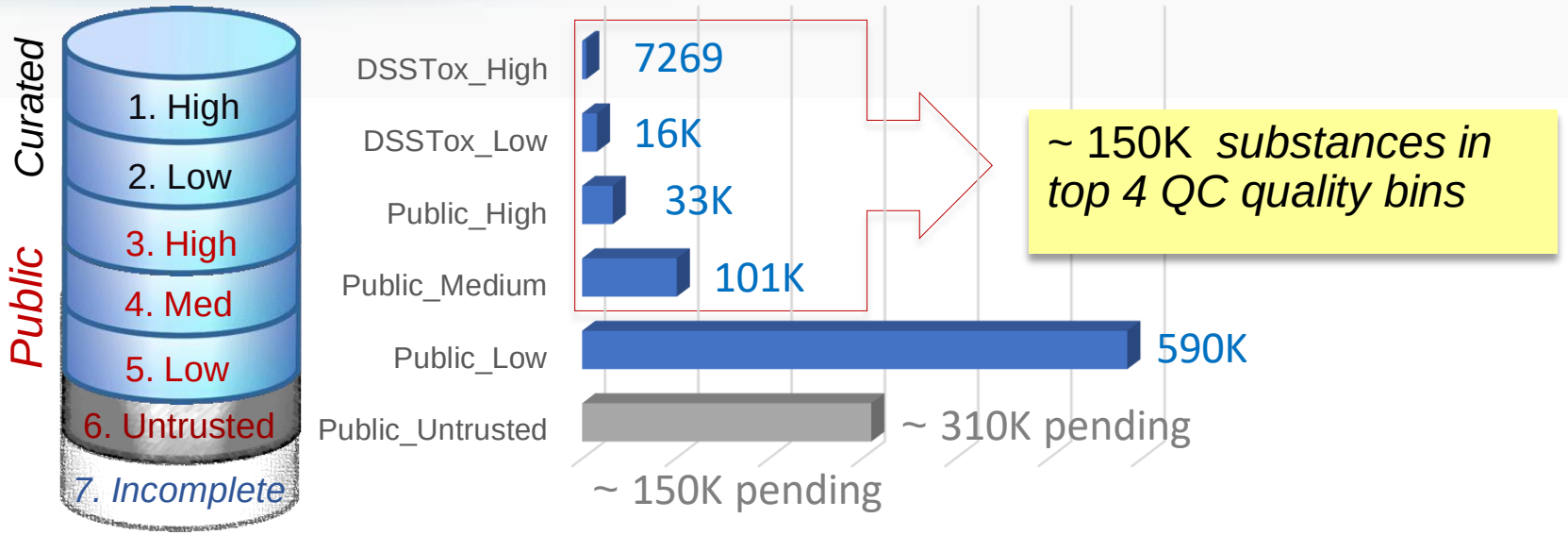


# Underneath the Dashboard



# Distribution of curated data
# Now at >910k substances




| 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 |

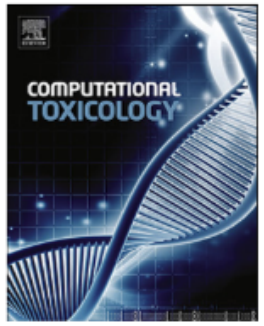
# A little more about our data quality

Computational Toxicology 12 (2019) 100096

Contents lists available at ScienceDirect

Computational Toxicology

journal homepage: www.elsevier.com/locate/comtox



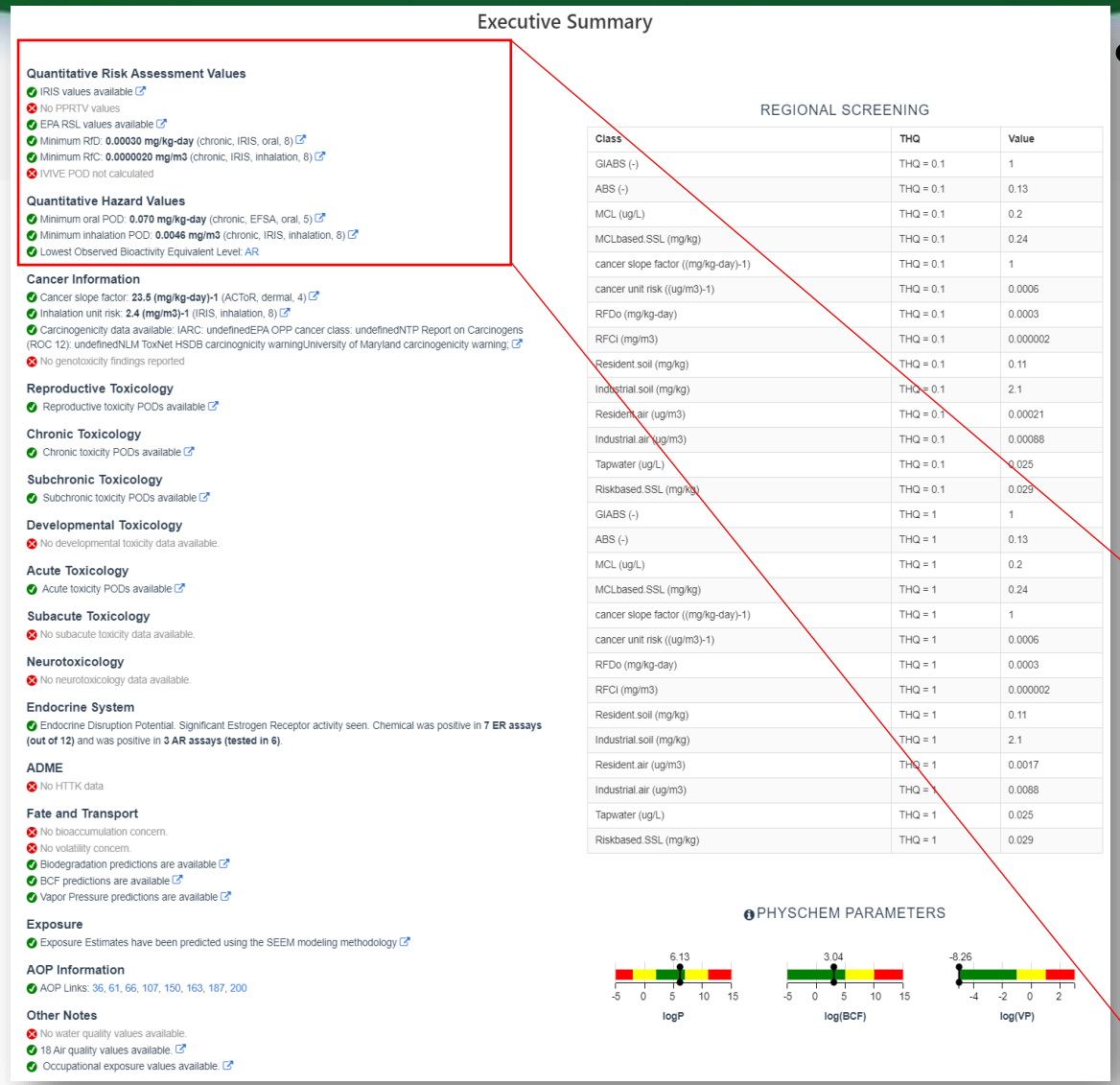

## EPA's DSSTox database: History of development of a curated chemistry resource supporting computational toxicology research

Christopher M. Grulke[a], Antony J. Williams[a], Inthirany Thillanadarajah[b], Ann M. Richard[a,*]

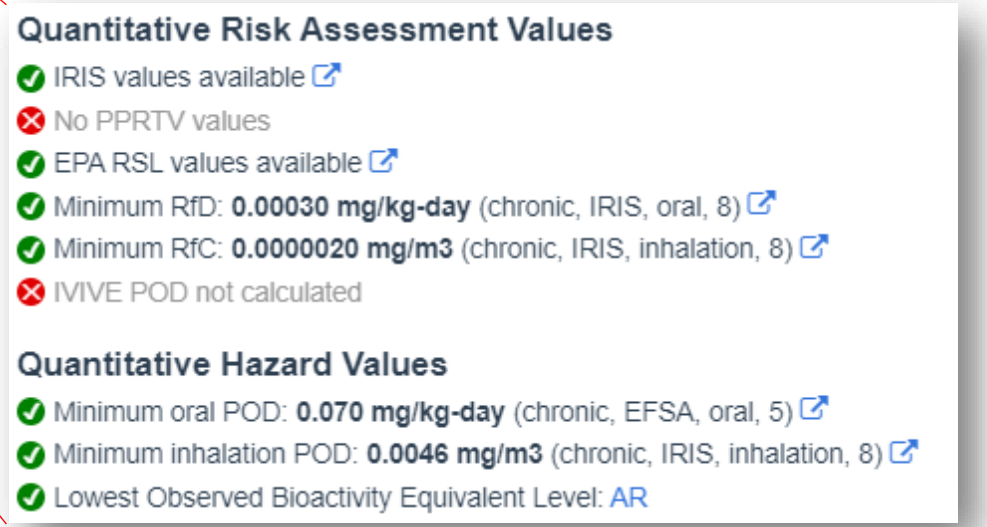
[a] National Center for Computational Toxicology, Office of Research & Development, US Environmental Protection Agency, Mail Drop D143-02, Research Triangle Park, NC 27711, USA

[b] Senior Environmental Employment Program, US Environmental Protection Agency, Research Triangle Park, NC 27711, USA

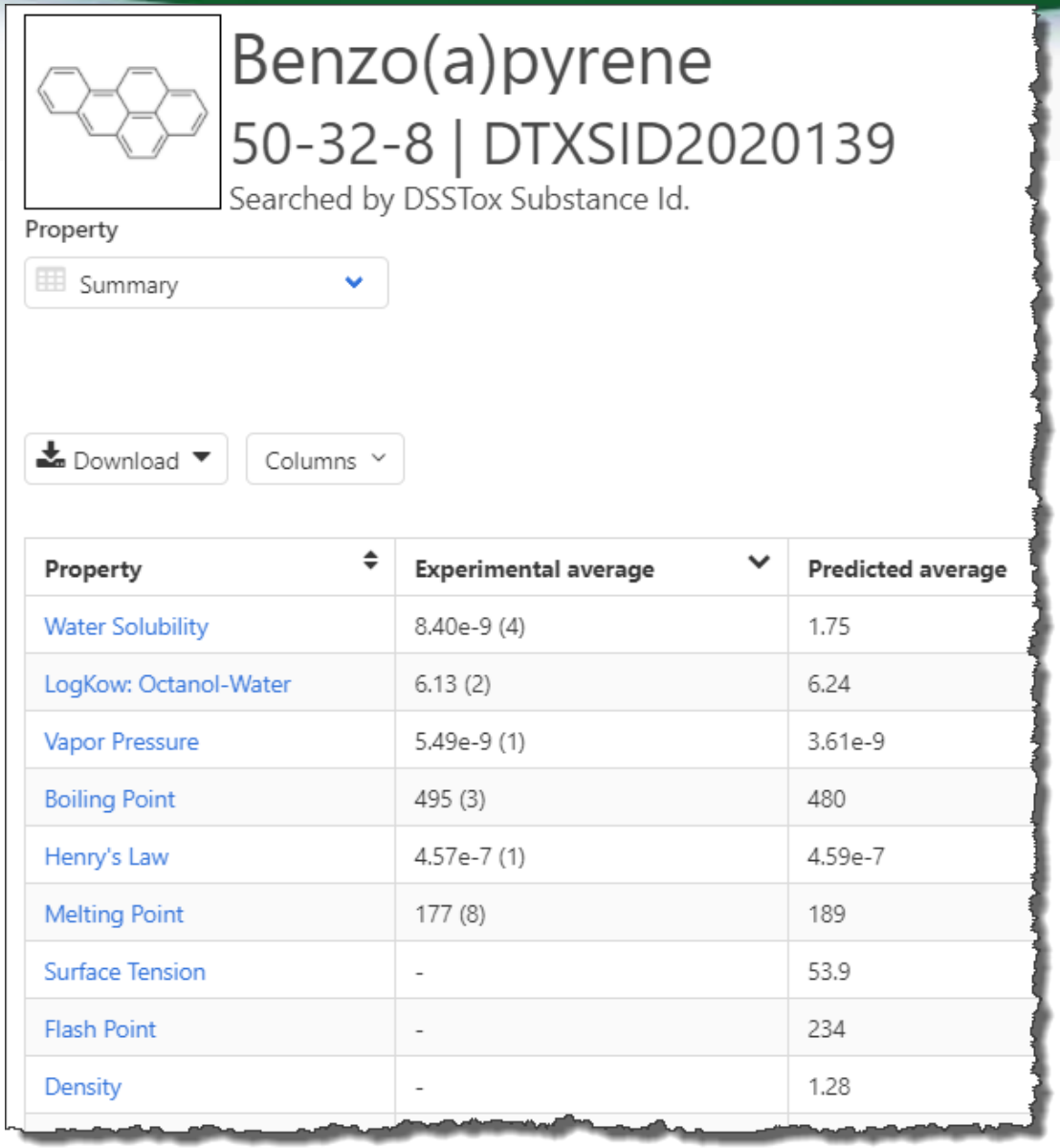
# “Executive Summary”




- Overview of toxicity-related info
  - Quantitative values
  - Info re. toxicology subsets
  - Physchem. and Fate & Transport
  - Adverse Outcome Pathway links
  - *In vitro* bioactivity summary plot



# Experimental and Predicted Data



Benzo(a)pyrene

50-32-8 | DTXSID2020139

Searched by DSSTox Substance Id.

Property

Summary

Download Columns

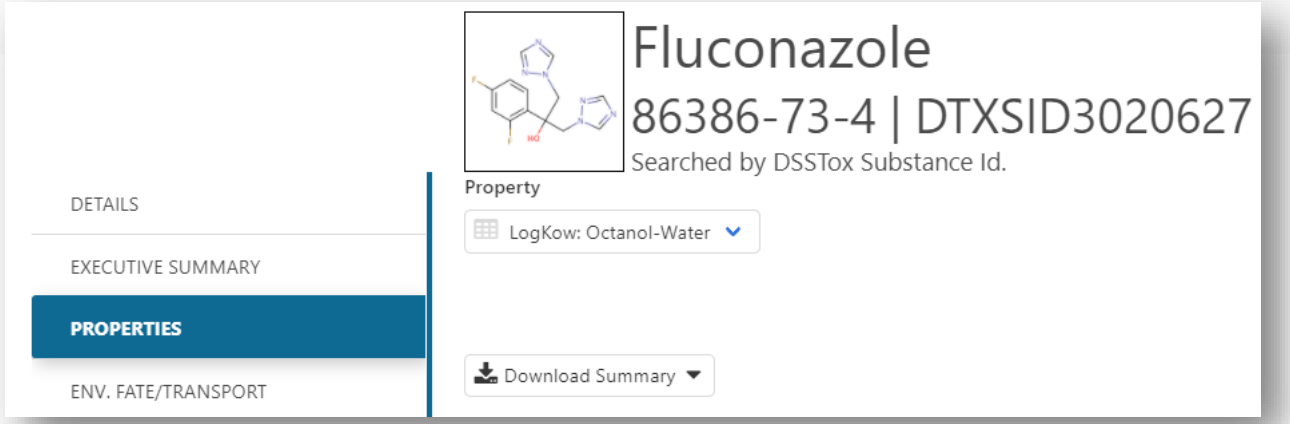
| Property | Experimental average | Predicted average |
|---|---|---|
| Water Solubility | 8.40e-9 (4) | 1.75 |
| LogKow: Octanol-Water | 6.13 (2) | 6.24 |
| Vapor Pressure | 5.49e-9 (1) | 3.61e-9 |
| Boiling Point | 495 (3) | 480 |
| Henry's Law | 4.57e-7 (1) | 4.59e-7 |
| Melting Point | 177 (8) | 189 |
| Surface Tension | - | 53.9 |
| Flash Point | - | 234 |
| Density | - | 1.28 |

- Physchem and Fate & Transport experimental and predicted data
- Data can be downloaded as Excel, TSV and CSV files
- Predictions: multiple algorithms
  - EPI Suite: Estimation Program Interface
  - ACD/Labs (commercial)
  - TEST: **T**oxicity **E**stimation **S**oftware **T**ool
  - OPERA: **OPE**n structure–activity/ property **R**elationship **A**pp

# Different QS(X)R predictions

- There are many different “QSAR-related” predictions available
  - QSPR: quantitative structure–**property** relationships
  - QSAR: quantitative structure–**activity** relationships
  - QSUR: quantitative structure-**use** relationships

# Access to Predictions




## Predicted

Download Predicted Data

| Source | Result | Calculation Details | QMRF |
|---|---|---|---|
| EPISUITE | 0.250 | Not Available | Not Available |
| ACD/Labs Consensus | 0.698 | Not Available | Not Available |
| ACD/Labs | 0.500 | Not Available | Not Available |
| OPERA | 0.501 | OPERA Model Report [Inside AD] | Available |

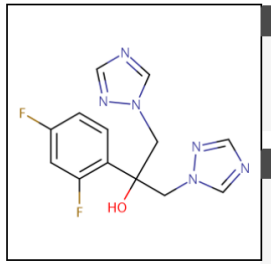
# OPERA Reports

OPERA Models: LogKow: Octanol-Water

## Fluconazole

86386-73-4 | DTXSID3020627

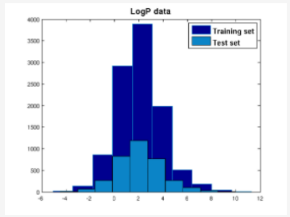
Print PDF

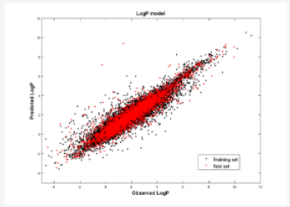


**Model Results**

**Predicted value:** 0.501
**Global applicability domain:** Inside
**Local applicability domain index:** 0.998
**Confidence level:** 0.732

**Model Performance**



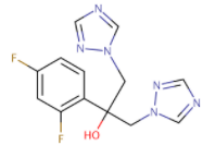
QMRF

Weighted KNN model

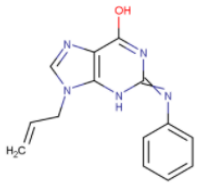
Weighted KNN model

| 5-fold CV (75%) | | Training (75%) | | Test (25%) | |
|---|---|---|---|---|---|
| Q2 | RMSE | R2 | RMSE | R2 | RMSE |
| 0.850 | 0.690 | 0.860 | 0.670 | 0.860 | 0.780 |

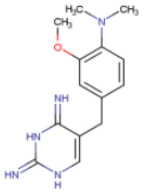
**Nearest Neighbors from the Training Set**



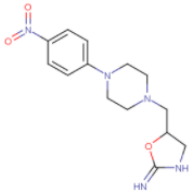
Fluconazole
Measured:0.5
Predicted: 0.50



GUANINEN2PHENYL9ALLYL
Measured:1.75
Predicted: 1.75

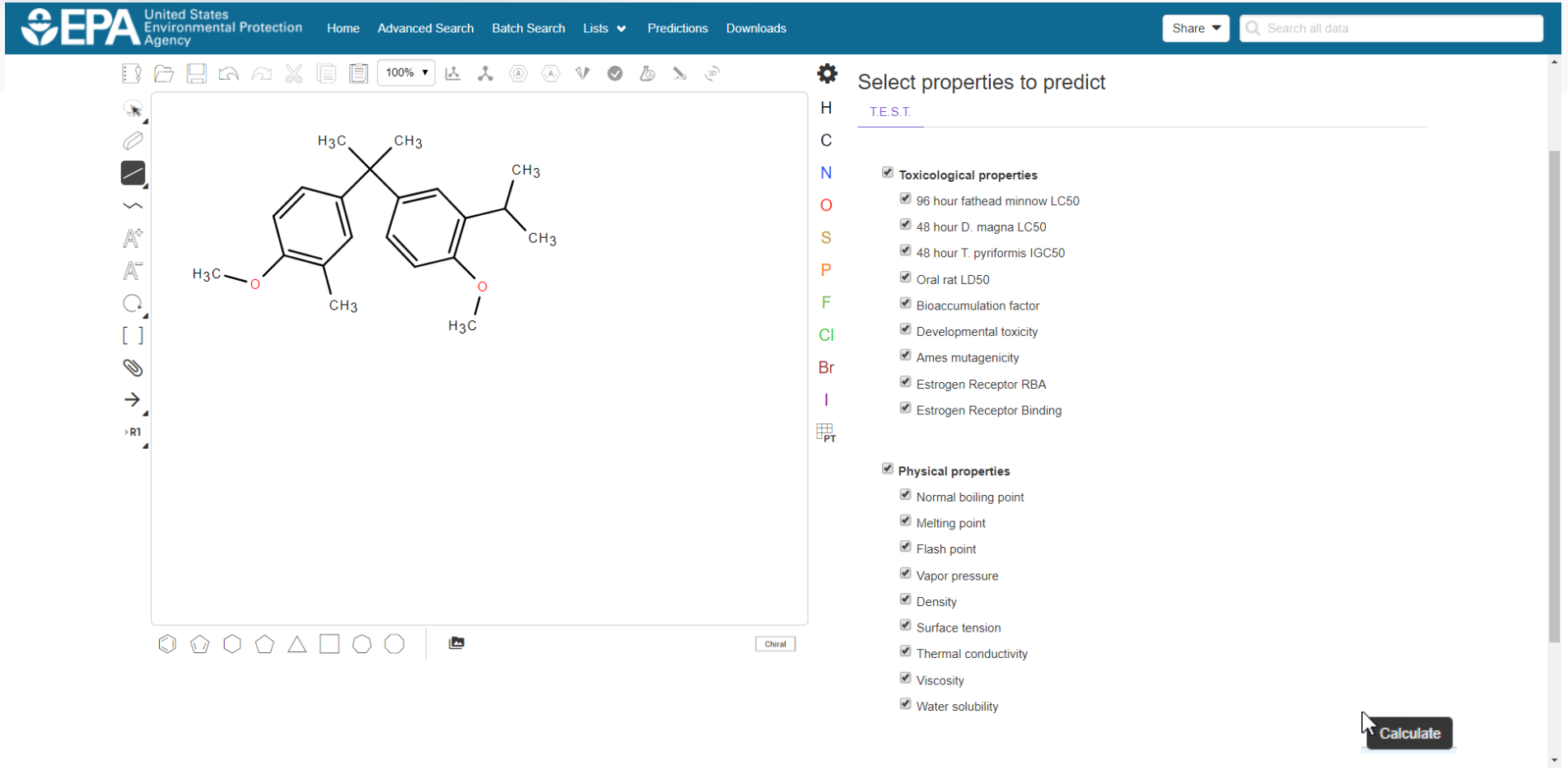


2,4-PYRIMIDINEDIAMINE, 5-[[4-(DIMETHYLAMINO)-3-M
Measured:1.87
Predicted: 1.87



5-(1-P-NITROPHENYL-4-PIPERAZINYL)METHYL-2-AMINO-
Measured:1.23
Predicted: 1.23

# Real-Time Predictions

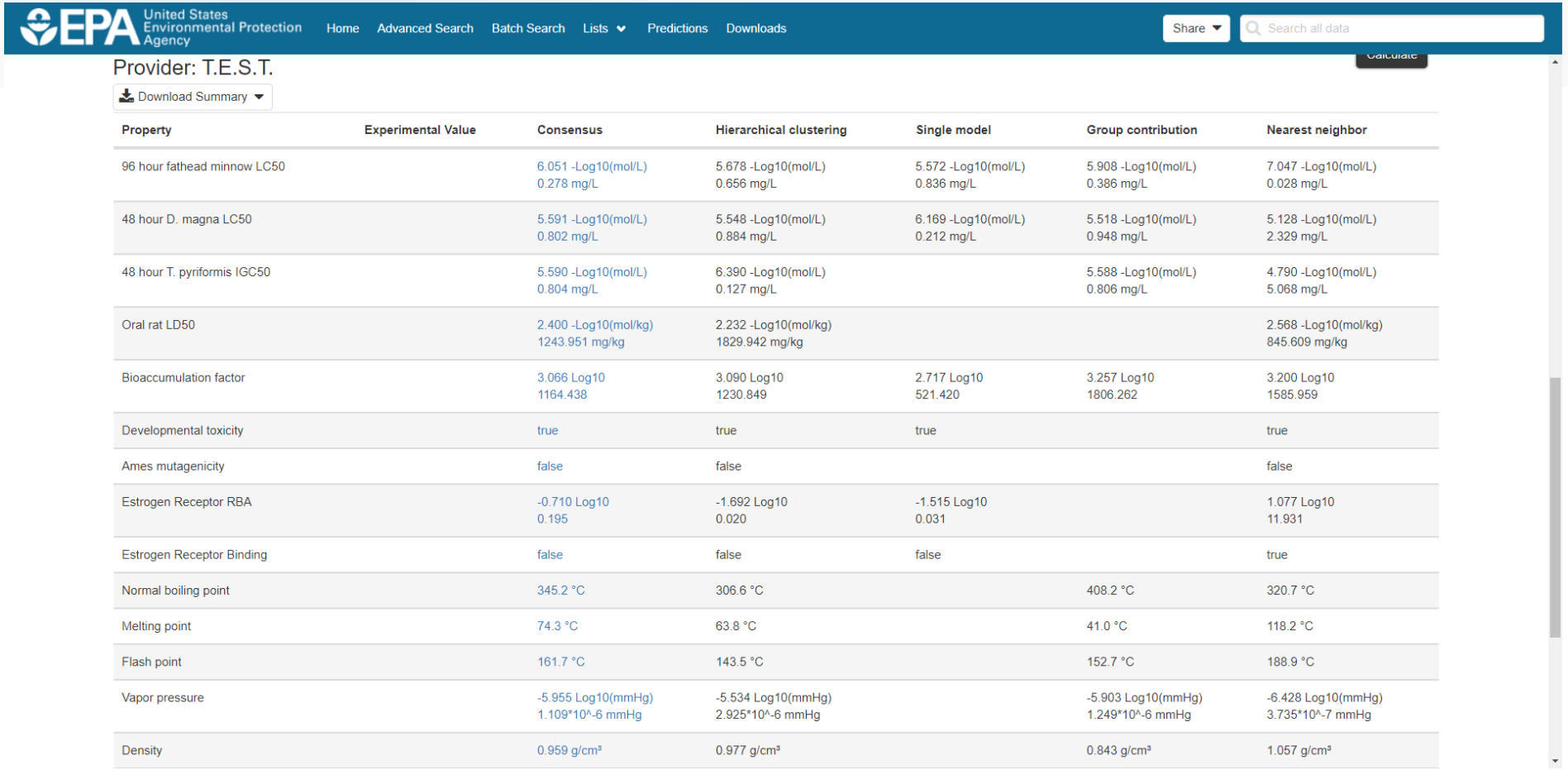


# Toxicity and Properties

- [x] Toxicological properties
  - [x] 96 hour fathead minnow LC50
  - [x] 48 hour D. magna LC50
  - [x] 48 hour T. pyriformis IGC50
  - [x] Oral rat LD50
  - [x] Bioconcentration factor
  - [x] Developmental toxicity
  - [x] Ames mutagenicity
  - [x] Estrogen Receptor RBA
  - [x] Estrogen Receptor Binding

- [x] Physical properties
  - [x] Normal boiling point
  - [x] Melting point
  - [x] Flash point
  - [x] Vapor pressure
  - [x] Density
  - [x] Surface tension
  - [x] Thermal conductivity
  - [x] Viscosity
  - [x] Water solubility

# Real-Time Predictions




| Property | Experimental Value | Consensus | Hierarchical clustering | Single model | Group contribution | Nearest neighbor |
|---|---|---|---|---|---|---|
| 96 hour fathead minnow LC50 | | 6.051 -Log10(mol/L)<br>0.278 mg/L | 5.678 -Log10(mol/L)<br>0.656 mg/L | 5.572 -Log10(mol/L)<br>0.836 mg/L | 5.908 -Log10(mol/L)<br>0.386 mg/L | 7.047 -Log10(mol/L)<br>0.028 mg/L |
| 48 hour D. magna LC50 | | 5.591 -Log10(mol/L)<br>0.802 mg/L | 5.548 -Log10(mol/L)<br>0.884 mg/L | 6.169 -Log10(mol/L)<br>0.212 mg/L | 5.518 -Log10(mol/L)<br>0.948 mg/L | 5.128 -Log10(mol/L)<br>2.329 mg/L |
| 48 hour T. pyriformis IGC50 | | 5.590 -Log10(mol/L)<br>0.804 mg/L | 6.390 -Log10(mol/L)<br>0.127 mg/L | | 5.588 -Log10(mol/L)<br>0.806 mg/L | 4.790 -Log10(mol/L)<br>5.068 mg/L |
| Oral rat LD50 | | 2.400 -Log10(mol/kg)<br>1243.951 mg/kg | 2.232 -Log10(mol/kg)<br>1829.942 mg/kg | | | 2.568 -Log10(mol/kg)<br>845.609 mg/kg |
| Bioaccumulation factor | | 3.066 Log10<br>1164.438 | 3.090 Log10<br>1230.849 | 2.717 Log10<br>521.420 | 3.257 Log10<br>1806.262 | 3.200 Log10<br>1585.959 |
| Developmental toxicity | | true | true | true | | true |
| Ames mutagenicity | | false | false | | | false |
| Estrogen Receptor RBA | | -0.710 Log10<br>0.195 | -1.692 Log10<br>0.020 | -1.515 Log10<br>0.031 | | 1.077 Log10<br>11.931 |
| Estrogen Receptor Binding | | false | false | false | | true |
| Normal boiling point | | 345.2 °C | 306.6 °C | | 408.2 °C | 320.7 °C |
| Melting point | | 74.3 °C | 63.8 °C | | 41.0 °C | 118.2 °C |
| Flash point | | 161.7 °C | 143.5 °C | | 152.7 °C | 188.9 °C |
| Vapor pressure | | -5.955 Log10(mmHg)<br>1.109*10^-6 mmHg | -5.534 Log10(mmHg)<br>2.925*10^-6 mmHg | | -5.903 Log10(mmHg)<br>1.249*10^-6 mmHg | -6.428 Log10(mmHg)<br>3.735*10^-7 mmHg |
| Density | | 0.959 g/cm³ | 0.977 g/cm³ | | 0.843 g/cm³ | 1.057 g/cm³ |

# How do we gather data for models

- We are continuously gathering data…where from?
  - How do we validate?
  - What can we check?

- Projects underway at present that may be of interest
  - Water Solubility dataset
  - Mass Spec Amenability
  - Eye and Skin Sensitization and Irritation
  - PFAS chemicals

# What do we use predictions for?

- Property predictions can be used for
  - Experimental design – what chemicals are too volatile to perform bioactivity screens on?
  - As inputs to other models – for example toxicokinetic models, exposure models (we cannot measure all the properties we need to build models)
  - To use as flags related to persistence and bioaccumulation

# Safety Data

GHS Data

Print Page

PUBCHEM > BENZO[A]PYRENE > LABORATORY CHEMICAL SAFETY SUMMARY (LCSS) > GHS CLASSIFICATION

CID 2336

## Benzo[a]pyrene

### GHS Classification

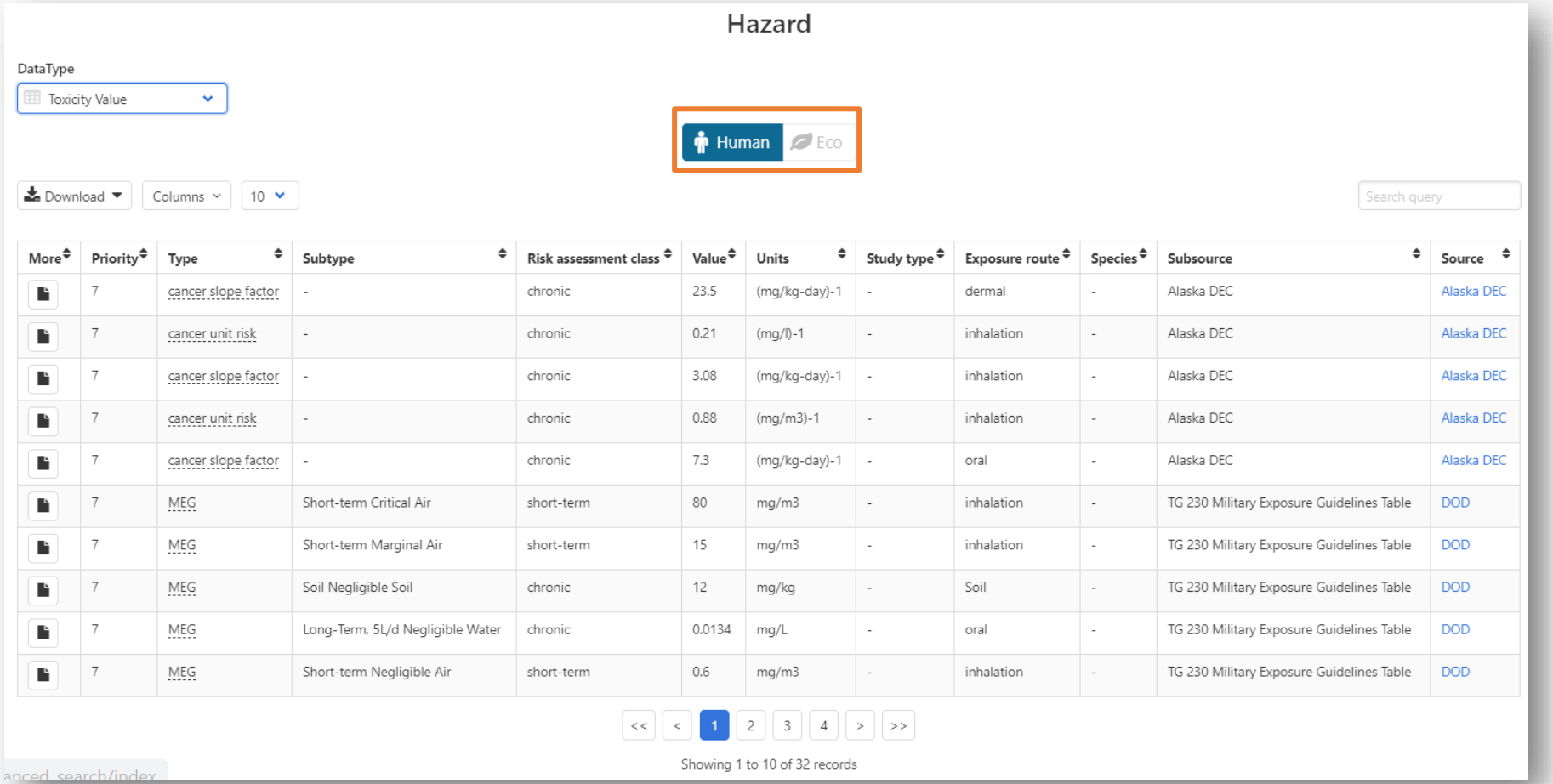
Showing 6 of 6

| | |
|---|---|
| **Pictogram(s)** |  Irritant, Health Hazard, Environmental Hazard |
| **Signal** | Danger |
| **GHS Hazard Statements** | H317: May cause an allergic skin reaction [Warning Sensitization, Skin]<br>H340: May cause genetic defects [Danger Germ cell mutagenicity]<br>H350: May cause cancer [Danger Carcinogenicity]<br>H360FD: May damage fertility; May damage the unborn child [Danger Reproductive toxicity]<br>H400: Very toxic to aquatic life [Warning Hazardous to the aquatic environment, acute hazard]<br>H410: Very toxic to aquatic life with long lasting effects [Warning Hazardous to the aquatic environment, long-term hazard] |
| **Precautionary Statement Codes** | P201, P202, P261, P272, P273, P280, P281, P302+P352, P308+P313, P321, P333+P313, P363, P391, P405, and P501<br>(The corresponding statement to each P-code can be found at the GHS Classification page.) |

# Chemical Hazard Data

## ToxVal Database

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




| More | Priority | Type | Subtype | Risk assessment class | Value | Units | Study type | Exposure route | Species | Subsource | Source |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | 7 | cancer slope factor | - | chronic | 23.5 | (mg/kg-day)-1 | - | dermal | - | Alaska DEC | Alaska DEC |
| | 7 | cancer unit risk | - | chronic | 0.21 | (mg/l)-1 | - | inhalation | - | Alaska DEC | Alaska DEC |
| | 7 | cancer slope factor | - | chronic | 3.08 | (mg/kg-day)-1 | - | inhalation | - | Alaska DEC | Alaska DEC |
| | 7 | cancer unit risk | - | chronic | 0.88 | (mg/m3)-1 | - | inhalation | - | Alaska DEC | Alaska DEC |
| | 7 | cancer slope factor | - | chronic | 7.3 | (mg/kg-day)-1 | - | oral | - | Alaska DEC | Alaska DEC |
| | 7 | MEG | Short-term Critical Air | short-term | 80 | mg/m3 | - | inhalation | - | TG 230 Military Exposure Guidelines Table | DOD |
| | 7 | MEG | Short-term Marginal Air | short-term | 15 | mg/m3 | - | inhalation | - | TG 230 Military Exposure Guidelines Table | DOD |
| | 7 | MEG | Soil Negligible Soil | chronic | 12 | mg/kg | - | Soil | - | TG 230 Military Exposure Guidelines Table | DOD |
| | 7 | MEG | Long-Term, 5L/d Negligible Water | chronic | 0.0134 | mg/L | - | oral | - | TG 230 Military Exposure Guidelines Table | DOD |
| | 7 | MEG | Short-term Negligible Air | short-term | 0.6 | mg/m3 | - | inhalation | - | TG 230 Military Exposure Guidelines Table | DOD |

# Let’s talk about Export Formats

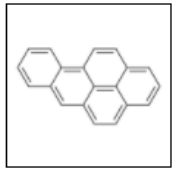
- Anywhere you see a table you can export
  - CSV is great for integration with other applications (plus read into Excel)
  - Excel file is generally the best for “viewing” as it can have multiple worksheets, color flagging of cells and offers all

- If you have cheminformatics tools SDF files are the best – view structures directly as concatenated “molfiles”

# Let’s Talk Exposure

- Types of Exposure Data on the Dashboard
  - Consumer product categories and uses
  - Products containing the chemical
  - Predicted exposure levels from modeling

# Sources of Exposure to Chemicals



## Benzo(a)pyrene

50-32-8 | DTXSID2020139

Searched by DSSTox Substance Id.

### Chemical Weight Fractions

Download | Columns | 10 | Search query

| Product Name | Product Use Category | Minimum Weight Fraction | Maximum Weight Fraction | Data Type | Source |
|---|---|---|---|---|---|
| m-525-1-5x pah mixtures 0.5 mg/ml for method 525 | Not Yet Categorized: | | | MSDS | SIRI |
| mm6125 surface conditioner | Not Yet Categorized: | | | Health Product Declaration | Health Product Declaration Collaborative |
| monolithic membrane 6125 (mm6125) / monolithic membrane | Not Yet Categorized: | | | Health Product Declaration | Health Product Declaration Collaborative |
| organic potablewatr pw 32_component h:reg semi-volatile 690 | Not Yet Categorized: | 0.00 | 1.00e-3 | MSDS | SIRI |
| polynuclear aromatic hydrocarbon mixture_ ep84627 | Not Yet Categorized: | | | MSDS | SIRI |
| prestone(r) power steering fluid | engine maintenance: auto fluids and additives | | | MSDS | CPCPdb |
| r-12 shield tite wet surface coating | Not Yet Categorized: | 0.00 | 0.500 | MSDS | SIRI |
| sea tar 1010_ 0028 | Not Yet Categorized: | | | MSDS | SIRI |
| supelpreme-hc kit pah mix_ 48909 | Not Yet Categorized: | | | MSDS | SIRI |
| supelpreme-hc pah mix 1ml_ 48905 | Not Yet Categorized: | | | MSDS | SIRI |

<< < 1 2 3 > >>

Showing 11 to 20 of 21 records

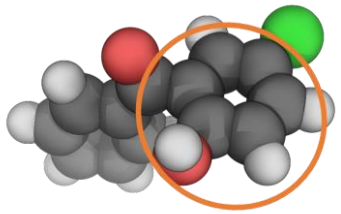
# Machine Learning NAMS

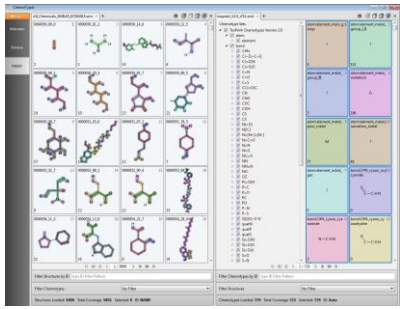
**Chemical Functional Use Database (FUSE)**

Positive Examples

Negative Examples

Chemical Structure and Property Descriptors






Successful Model

Failed Model

Probabilistic Predictions of Potential Chemical Uses

Phillips *et al.* (2017)

# QSUR modeling

EPA United States Environmental Protection Agency

## High-throughput screening of chemicals as functional substitutes using structure-based classification models†

Check for updates

Katherine A. Phillips, *[ac] John F. Wambaugh,[b] Christopher M. Grulke,[b] Kathie L. Dionisio[c] and Kristin K. Isaacs[c]

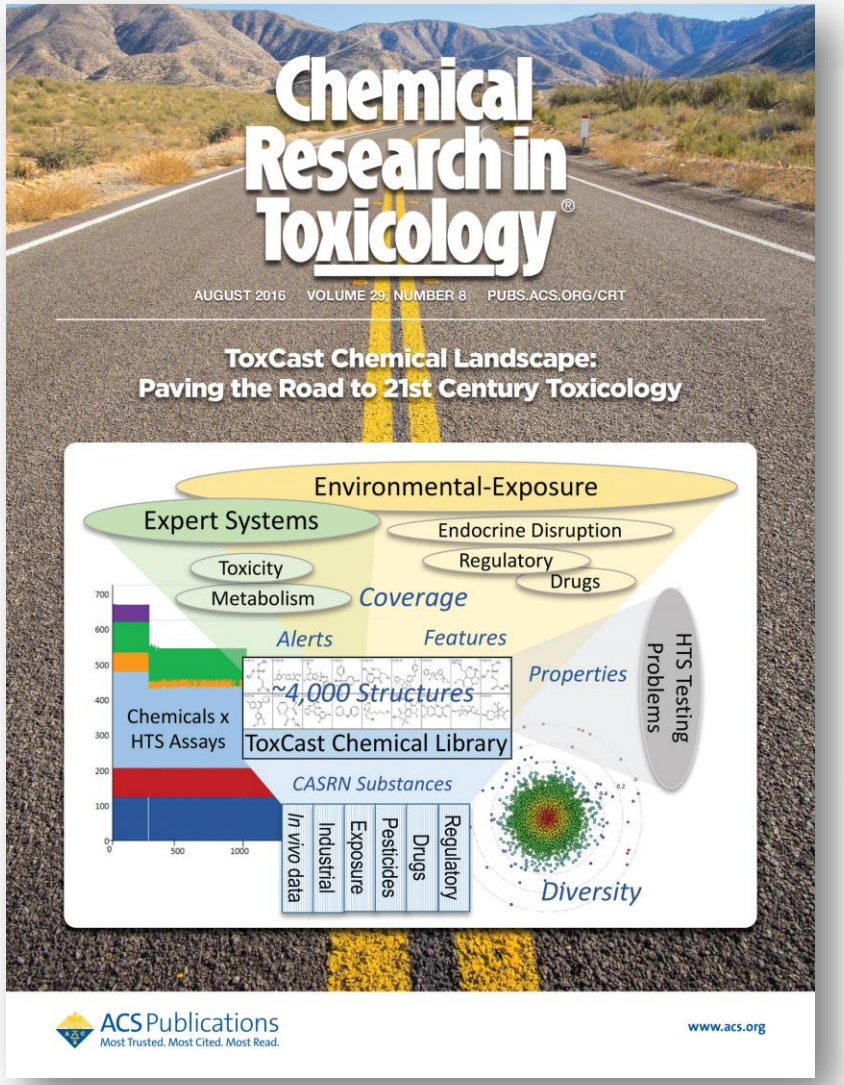
Predicted Probability of Associated Functional Use
QSAR Version/Date: 2015-11-06

Download 10

| Harmonized functional use | Probability |
|---|---|
| preservative | 0.988 |
| UV absorber | 0.885 |
| fragrance | 0.653 |
| antioxidant | 0.608 |
| skin conditioner | 0.475 |
| skin protectant | 0.411 |
| chelator | 0.364 |
| colorant | 0.285 |
| antimicrobial | 0.279 |
| crosslinker | 0.187 |

# ToxCast

EPA United States Environmental Protection Agency



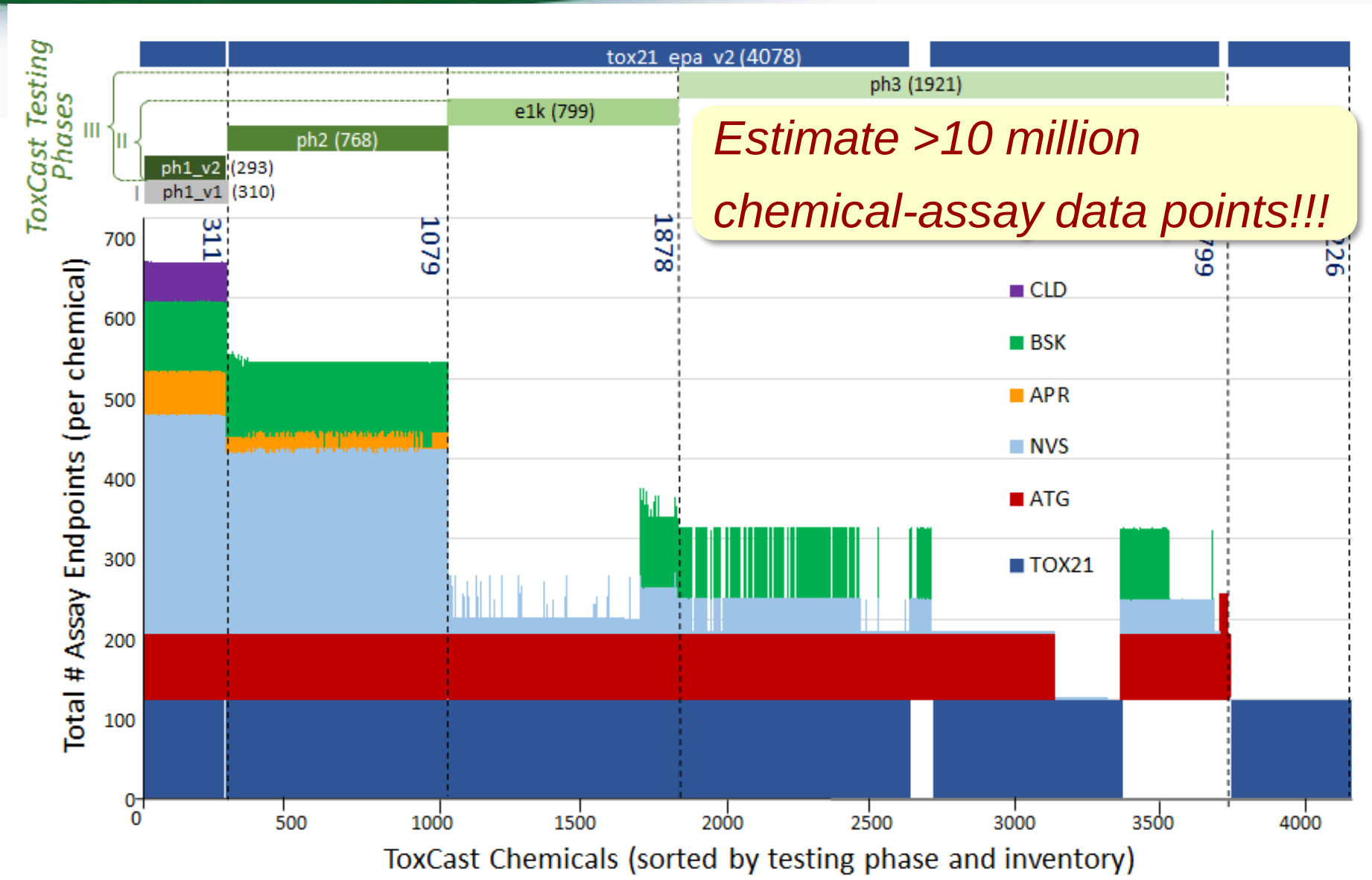

## ToxCast Chemical Landscape: Paving the Road to 21st Century Toxicology

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

View Author Information

**Cite this:** *Chem. Res. Toxicol.* 2016, 29, 8, 1225–1251
Publication Date: July 1, 2016
https://doi.org/10.1021/acs.chemrestox.6b00135

# ToxCast/To21 HTS data



# ToxCast Chemicals and Assays

EPA United States Environmental Protection Agency

## Select List

Download | Columns | toxcast_ | Copy Filtered Lists URL

| List Acronym | List Name | Last Updated | Number of Chemicals | List Description |
|---|---|---|---|---|
| TOXCAST_PH1V2 | TOXCAST_ph1v2 - EPA ToxCast Screening Library (ph1v2 Subset) | 2016-01-25 | 293 | TOXCAST_ph1v2 is the ph1v2 subset of TOXCAST, a reprocured subset of Phase I (ph1v1) chemicals moved into Phase II and later testing phases of the ToxCast program. |
| TOXCAST_PHASEI | TOXCAST_Phasei - EPA ToxCast Screening Library (Phase I subset) | 2016-01-29 | 310 | TOXCAST_PhaseI corresponds to the ph1v1 subset of TOXCAST (mostly pesticides) screened in Phase I of the ToxCast program. |
| TOXCAST_PH2 | TOXCAST_ph2 - EPA ToxCast Screening Library (ph2 Subset) | 2016-01-25 | 768 | TOXCAST_ph2 is the ph2 subset of TOXCAST, added in Phase II of the ToxCast program to increase chemical diversity and coverage of chemicals of concern to EPA programs. |
| TOXCAST_E1K | TOXCAST_e1k - EPA ToxCast Screening Library (e1k Subset) | 2016-01-25 | 799 | TOXCAST_e1k is the e1k subset of TOXCAST, selected for screening in endocrine-related assays. |
| TOXCAST_PHASEII | TOXCASST_PhaseII - EPA ToxCast Screening Library (Phase II Subset) | 2016-01-29 | 1864 | TOXCAST_PhaseII is the full set of chemicals screened in Phase II of the ToxCast program, consisting of TOXCAST_ph1v2, ph2 and e1k sublists. |
| TOXCAST_PH3 | TOXCAST_ph3 - EPA ToxCast Screening Library (ph3 subset) | 2018-04-11 | 2678 | TOXCAST_ph3 is the ph3 subset of TOXCAST, added to the most recent Phase III of the ToxCast program to further increase chemical diversity and coverage of chemicals of concern to EPA programs. |
| TOXCAST_PHASEIII | TOXCAST_PhaseIII - EPA ToxCast Screening Library (Phase II Subset) | 2017-04-11 | 4584 | TOXCAST_PhaseIII is the full set of chemicals available for screening in Phase III of the ToxCast program, consisting of the majority of chemicals screened in Phase II and newly added ph3 |

# ToxCast covers a lot of biology but not all ToxCast is growing over time.

EPA United States Environmental Protection Agency

*Invitrodb version 3.3 (released August 2020) contained **17 different assay sources**, covering (at least) **491 unique gene-related** targets with **1600 unique** assay endpoints.*

| Assay source | Long name | Truncated assay source description | Some rough notes on the biology covered |
|---|---|---|---|
| ACEA | ACEA Biosciences | real-time, label-free, cell growth assay system based on a microelectronic impedance readout | Endocrine (ER-induced proliferation) |
| APR | Apredica | CellCiphr High Content Imaging system | Hepatic cells (HepG2) |
| ATG | Attagene | multiplexed pathway profiling platform | Nuclear receptor and stress response profile |
| BSK | Bioseek | BioMAP system providing uniquely informative biological activity profiles in complex human primary co-culture systems | Immune/inflammation responses |
| NVS | Novascreen | large diverse suite of cell-free binding and biochemical assays. | Receptor binding; transporter protein binding; ion channels; enzyme inhibition; many targets |
| OT | Odyssey Thera | novel protein:protein interaction assays using protein-fragment complementation technology | Endocrine (ER and AR) |
| TOX21 | Tox21/NCGC | Tox21 is an interagency agreement between the NIH, NTP, FDA and EPA. NIH Chemical Genomics Center (NCGC) is the primary screening facility running ultra high-throughput screening assays across a large interagency-developed chemical library | Many – with many nuclear receptors |
| CEETOX | Ceetox/OpAns | HT-H295R assay | Endocrine (steroidogenesis) |
| CLD | CellzDirect | Formerly CellzDirect, this Contract Research Organization (CRO) is now part of the Invitrogen brand of Thermo Fisher providing cell-based in vitro assay screening services using primary hepatocytes. | Liver (Phase I/Phase II/ Phase III expression) |
| NHEERL_PADILLA | NHEERL Padilla Lab | The Padilla laboratory at the EPA National Health and Environmental Effects Research Laboratory focuses on the development and screening of zebrafish assays. | Zebrafish terata |
| NCCT | NCCT Simmons Lab | The Simmons Lab at the EPA National Center for Computational Toxicology focuses on developing and implementing in vitro methods to identify potential environmental toxicants. | Endocrine (thyroid - thyroperoxidase inhibition) |
| TANGUAY | Tanguay Lab | The Tanguay Lab, based at the Oregon State University Sinnhuber Aquatic Research Laboratory, uses zebrafish as a systems toxicology model. | Zebrafish terata/phenotypes |
| NHEERL_NIS | NHEERL Stoker & Laws | The Stoker and Laws laboratories at the EPA National Health and Environmental Effects Research Laboratory work on the development and implementation of high-throughput assays, particularly related to the sodium-iodide cotransporter (NIS). | Endocrine (thyroid - NIS inhibition) |
| UPITT | University of Pittsburgh | The Johnston Lab at the University of Pittsburgh ran androgen receptor nuclear translocation assays under a Material Transfer Agreement (MTA) for the ToxCast Phase 1, Phase 2, and E1K chemicals. | Endocrine (AR related) |

# The Tox21 Screening Library

EPA United States Environmental Protection Agency

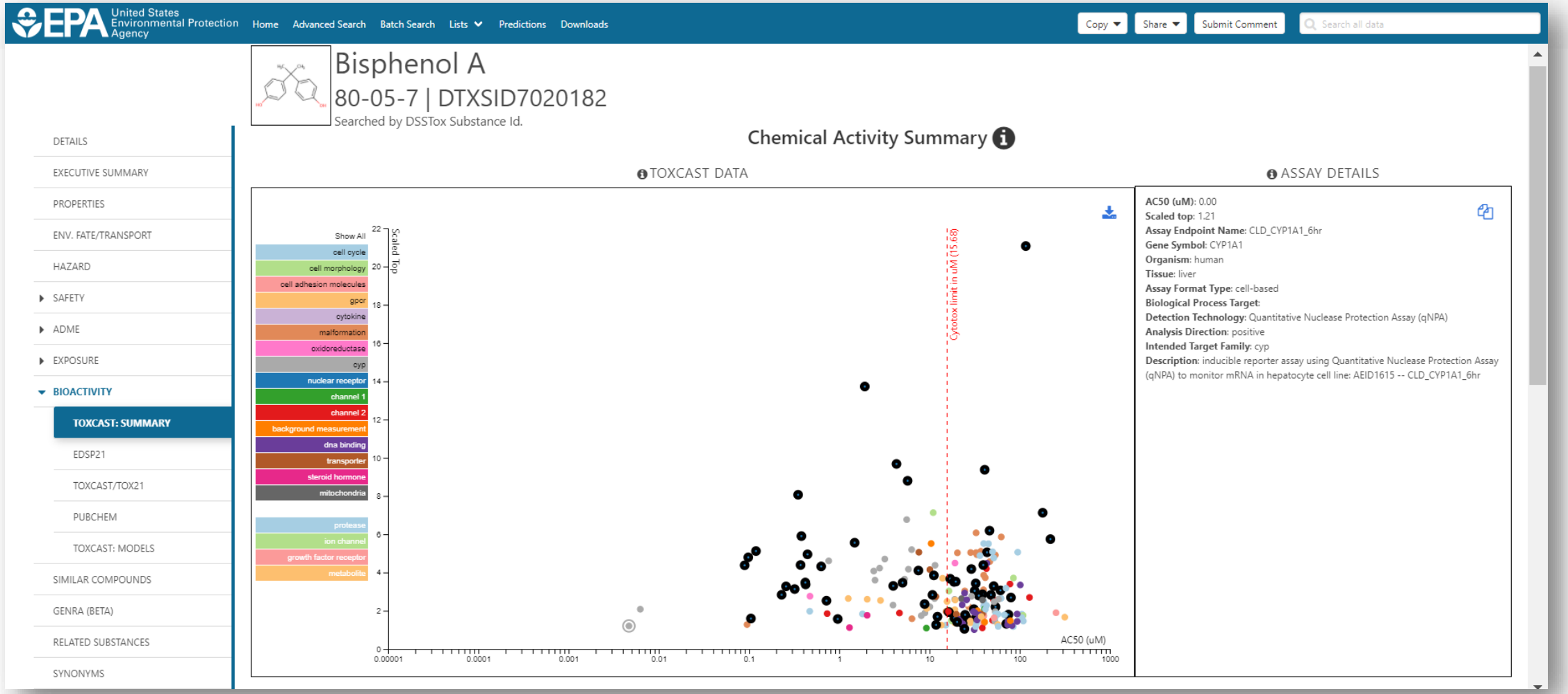
## Select List

Download | Columns | tox21 | Copy Filtered Lists URL

| List Acronym | List Name | Last Updated | Number of Chemicals | List Description |
|---|---|---|---|---|
| EPACHEMINV_AVAIL | CHEMINV; ToxCast/Tox21 Chemical inventory available as DMSO solutions (20181123) | 2018-11-21 | 6408 | EPACHEMINV_AVAIL is list of unique DSSTox substances available as DMSO solutions for ToxCast and Tox21 partner projects, managed by EPA Chemical Contract Services. |
| TOX21SL | TOX21SL: Tox21 Screening Library | 2017-02-23 | 8947 | TOX21SL is list of unique substances comprising the screening library for the Tox21 program, a multi-federal agency collaborative among the US EPA, NIH/NTP, NIH/NCATS, and the US FDA. |

2 records

# Let's look at the data



# Rich data tables – full transparency

217 active of 1152 assays

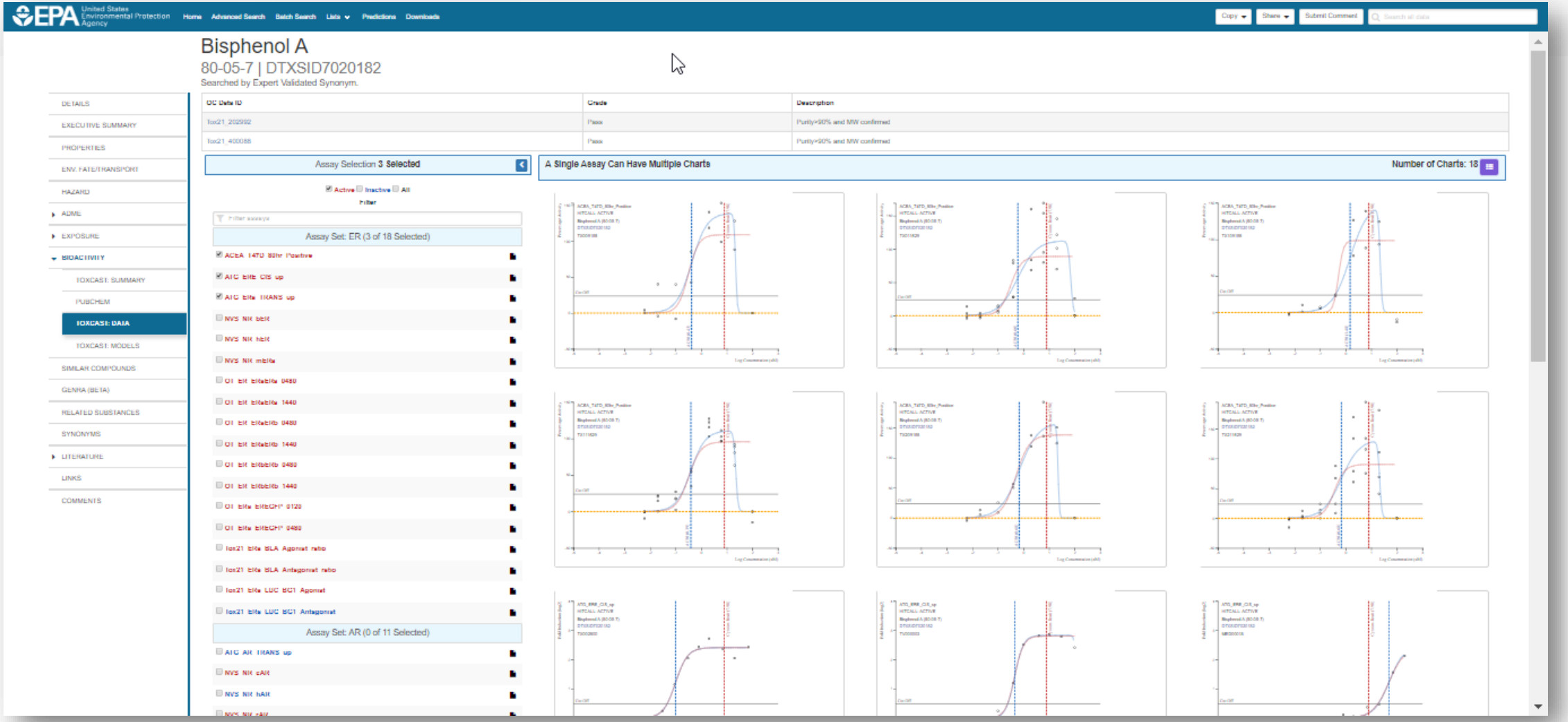
Download | Columns | 10 | Search query | Show Inactive | Show Background

| Name | Modal | SeqAPASS | Gene Symbol | Gene Name | AOP | Event | Hit Call | Top | Scaled Top | AC50 | logAC50 | Bmad | Cutoff | Intended Target Family |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| ATG_Xbp1_CIS_up | | NP_005071.2 | XBP1 | X-box binding protein 1 | - | - | ACTIVE | 1.08 | 1.83 | 93.8 | 1.97 | 0.118 | 0.590 | dna binding |
| ATG_VDRE_CIS_up | | NP_000367.1 | VDR | vitamin D (1,25- dihydroxyvitamin D3) receptor | - | - | ACTIVE | 1.71 | 2.35 | 8.84 | 0.946 | 0.146 | 0.728 | nuclear receptor |
| BSK_hDFCGF_VCAM1_down | | NP_001069.1 | VCAM1 | vascular cell adhesion molecule 1 | - | - | ACTIVE | 0.248 | 1.72 | 40.0 | 1.60 | 4.81e-2 | 0.144 | cell adhesion molecules |
| BSK_LPS_VCAM1_down | | NP_001069.1 | VCAM1 | vascular cell adhesion molecule 1 | - | - | ACTIVE | 0.107 | 1.35 | 40.0 | 1.60 | 2.31e-2 | 7.92e-2 | cell adhesion molecules |
| TOX21_p53_BLA_p2_ratio | | NP_000537.3 | TP53 | tumor protein p53 | - | - | ACTIVE | 35.5 | 1.78 | 73.7 | 1.87 | 0.959 | 20.0 | dna binding |
| TOX21_p53_BLA_p4_ratio | | NP_000537.3 | TP53 | tumor protein p53 | - | - | ACTIVE | 28.6 | 1.43 | 73.8 | 1.87 | 1.02 | 20.0 | dna binding |
| ATG_p53_CIS_dn | | NP_000537.3 | TP53 | tumor protein p53 | - | - | ACTIVE | 0.789 | 1.23 | 82.4 | 1.92 | 0.129 | 0.643 | dna binding |
| NVS_MP_rPBR | | NP_036647.1 | Tspo | translocator protein | - | - | ACTIVE | 61.5 | 1.96 | 15.3 | 1.19 | 5.24 | 31.4 | transporter |
| ATG_AP_2_CIS_dn | | NP_003211.1 | TFAP2A | transcription factor AP-2 alpha (activating enhancer binding protein 2 alpha) | - | - | ACTIVE | 0.458 | 1.44 | 93.8 | 1.97 | 6.35e-2 | 0.317 | dna binding |
| ATG_TCF_b_cat_CIS_dn | | NP_003193.2 | TCF7 | transcription factor 7 (T-cell specific, HMG-box) | - | - | ACTIVE | 1.34 | 1.96 | 30.7 | 1.49 | 0.137 | 0.687 | dna binding |

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

# Bioactivity Data (ToxCast/Tox21)

*Data below for Bisphenol A*



# #Actives for a chemical

EPA United States Environmental Protection Agency

217 active of 1152 assays

Download | Columns | 10 | Search query | Show Inactive | Show Background

| Name | Modal | SeqAPASS | Gene Symbol | Gene Name | AOP | Event | Hit Call | Top | Scaled Top | AC50 | logAC50 | Bmad | Cutoff | Intended Target Family |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| ATG_Xbp1_CIS_up | | NP_005071.2 | XBP1 | X-box binding protein 1 | - | - | ACTIVE | 1.08 | 1.83 | 93.8 | 1.97 | 0.118 | 0.590 | dna binding |
| ATG_VDRE_CIS_up | | NP_000367.1 | VDR | vitamin D (1,25- dihydroxyvitamin D3) receptor | - | - | ACTIVE | 1.71 | 2.35 | 8.84 | 0.946 | 0.146 | 0.728 | nuclear receptor |
| BSK_hDFCGF_VCAM1_down | | NP_001069.1 | VCAM1 | vascular cell adhesion molecule 1 | - | - | ACTIVE | 0.248 | 1.72 | 40.0 | 1.60 | 4.81e-2 | 0.144 | cell adhesion molecules |
| BSK_LPS_VCAM1_down | | NP_001069.1 | VCAM1 | vascular cell adhesion molecule 1 | - | - | ACTIVE | 0.107 | 1.35 | 40.0 | 1.60 | 2.31e-2 | 7.92e-2 | cell adhesion molecules |
| TOX21_p53_BLA_p2_ratio | | NP_000537.3 | TP53 | tumor protein p53 | - | - | ACTIVE | 35.5 | 1.78 | 73.7 | 1.87 | 0.959 | 20.0 | dna binding |
| TOX21_p53_BLA_p4_ratio | | NP_000537.3 | TP53 | tumor protein p53 | - | - | ACTIVE | 28.6 | 1.43 | 73.8 | 1.87 | 1.02 | 20.0 | dna binding |
| ATG_p53_CIS_dn | | NP_000537.3 | TP53 | tumor protein p53 | - | - | ACTIVE | 0.789 | 1.23 | 82.4 | 1.92 | 0.129 | 0.643 | dna binding |
| NVS_MP_rPBR | | NP_036647.1 | Tspo | translocator protein | - | - | ACTIVE | 61.5 | 1.96 | 15.3 | 1.19 | 5.24 | 31.4 | transporter |
| ATG_AP_2_CIS_dn | | NP_003211.1 | TFAP2A | transcription factor AP-2 alpha (activating enhancer binding protein 2 alpha) | - | - | ACTIVE | 0.458 | 1.44 | 93.8 | 1.97 | 6.35e-2 | 0.317 | dna binding |
| ATG_TCF_b_cat_CIS_dn | | NP_003193.2 | TCF7 | transcription factor 7 (T-cell specific, HMG-box) | - | - | ACTIVE | 1.34 | 1.96 | 30.7 | 1.49 | 0.137 | 0.687 | dna binding |

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

# Cytotoxicity Threshold


Volume 152, Issue 2
August 2016

**Editor's Highlight: Analysis of the Effects of Cell Stress and Cytotoxicity on *In Vitro* Assay Activity Across a Diverse Chemical and Assay Space** FREE

Richard Judson ✉, Keith Houck, Matt Martin, Ann M. Richard, Thomas B. Knudsen, Imran Shah, Stephen Little, John Wambaugh, R. Woodrow Setzer, Parth Kothya ... Show more

EPA United States Environmental Protection Agency

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Searched by DS

- DETAILS
- EXECUTIVE SUMMARY
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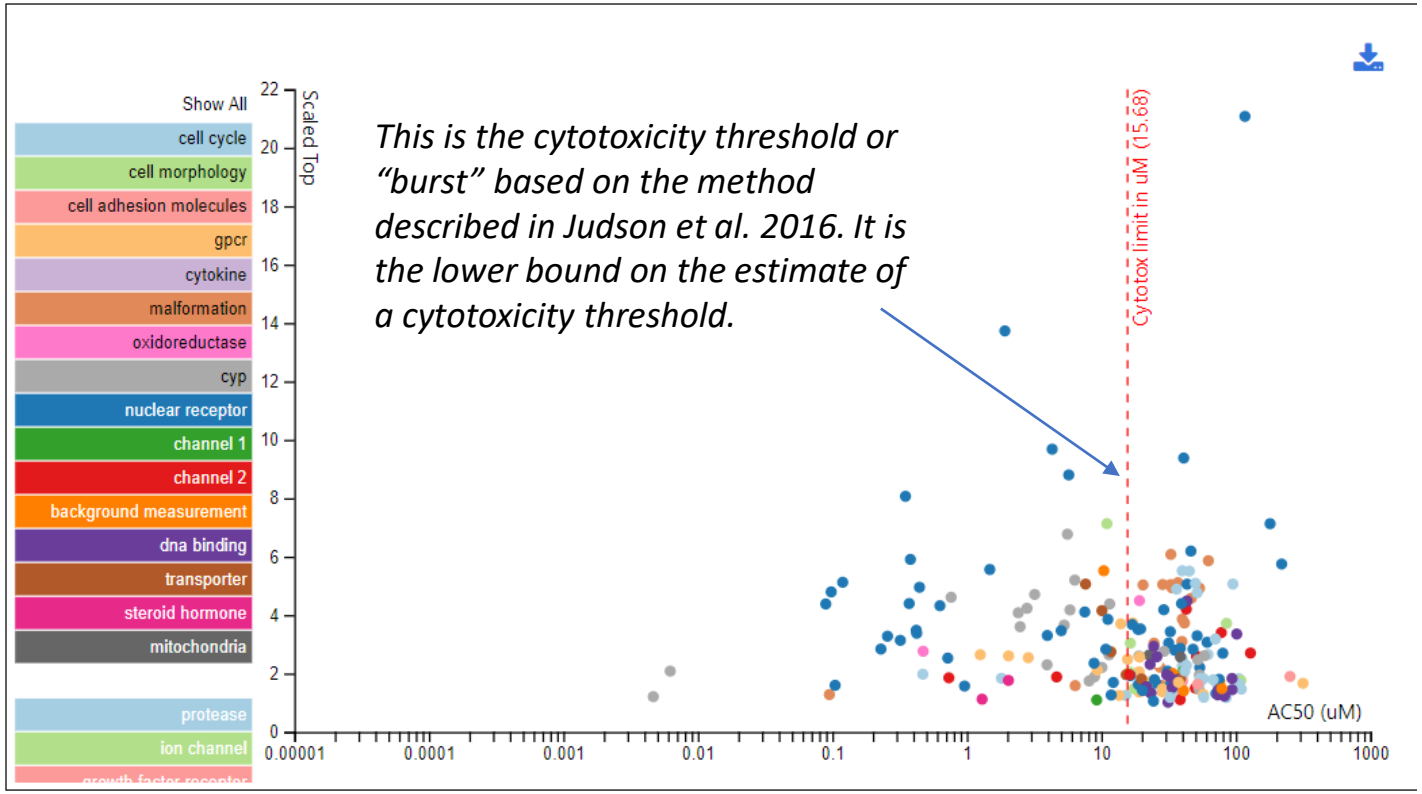
- SAFETY
- ADME
- EXPOSURE
- BIOACTIVITY
  - TOXCAST: SUMMARY
  - EDSP21
  - TOXCAST/TOX21
  - PUBCHEM
  - TOXCAST: MODELS

TOXCAST DATA

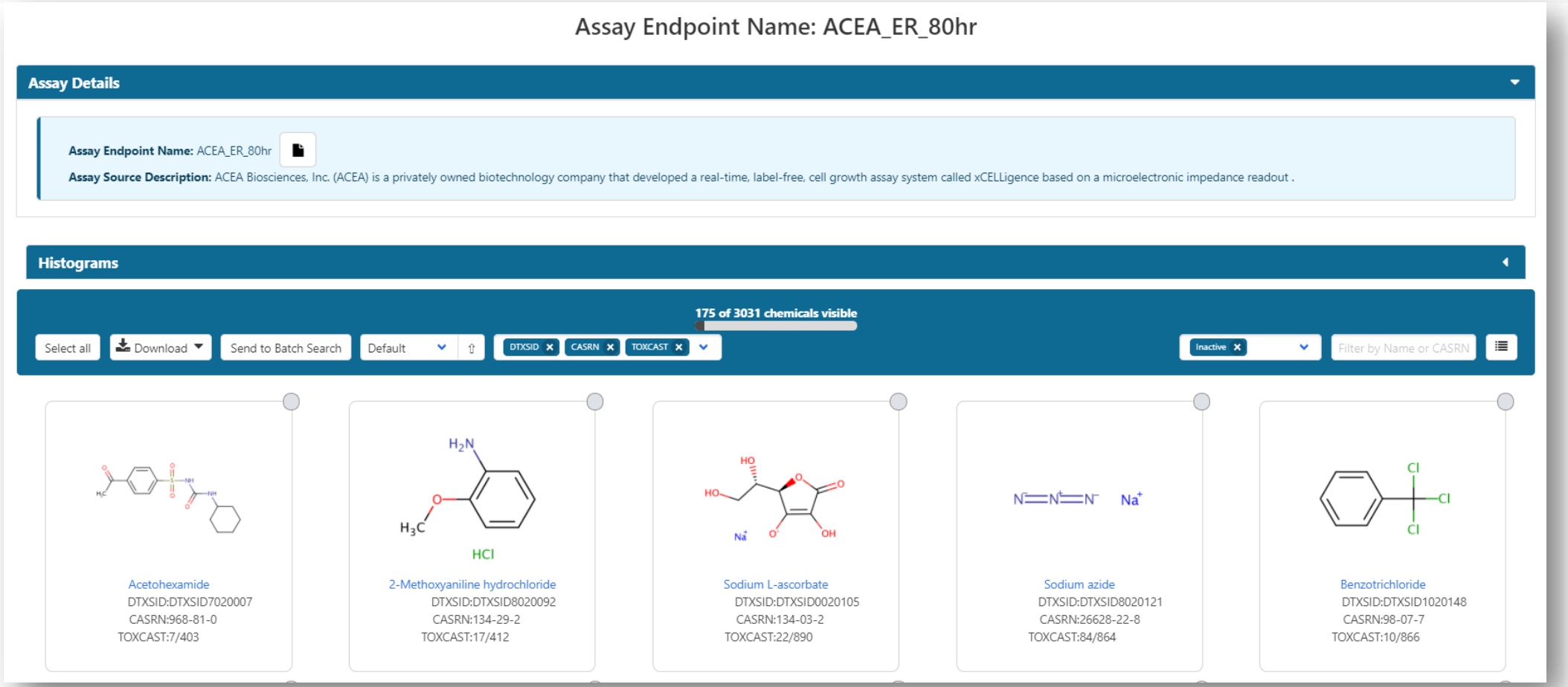



*This is the cytotoxicity threshold or "burst" based on the method described in Judson et al. 2016. It is the lower bound on the estimate of a cytotoxicity threshold.*

# What to make of the data

- Bisphenol A clearly has some *in vitro* nuclear receptor activity at concentrations that may be below or near cytotoxicity.
  - It has moderate ToxCast ER agonist and AR antagonist scores.
  - The cytotoxicity threshold or “burst” seems to support selectivity of some nuclear receptor responses.
  - Diving a little deeper into the intended target family supports this analysis.

# Let's look at the assay table ACEA_ER



# High-Level Visualizations of Data

EPA United States Environmental Protection Agency

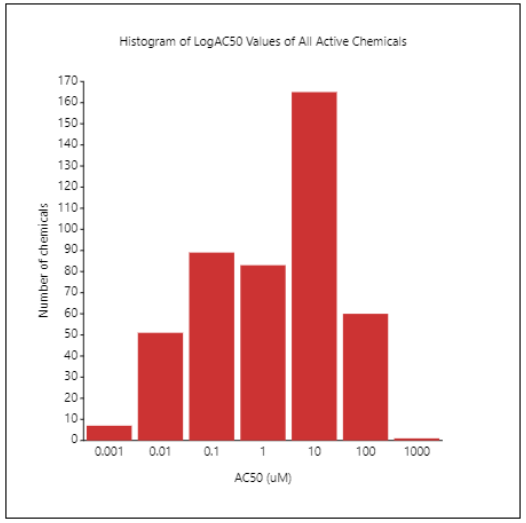
Assay Endpoint Name: ACEA_ER_80hr

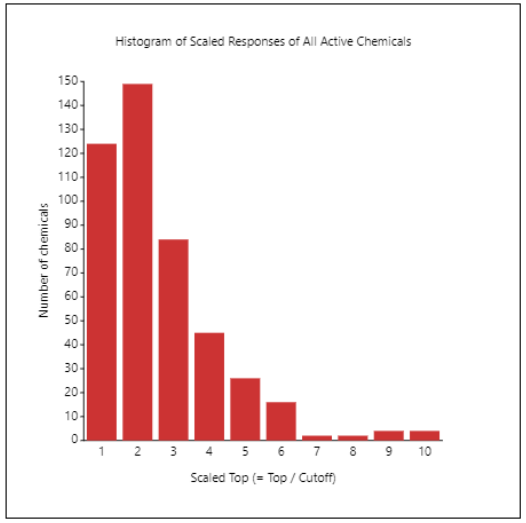
**Assay Details**

**Assay Endpoint Name:** ACEA_ER_80hr

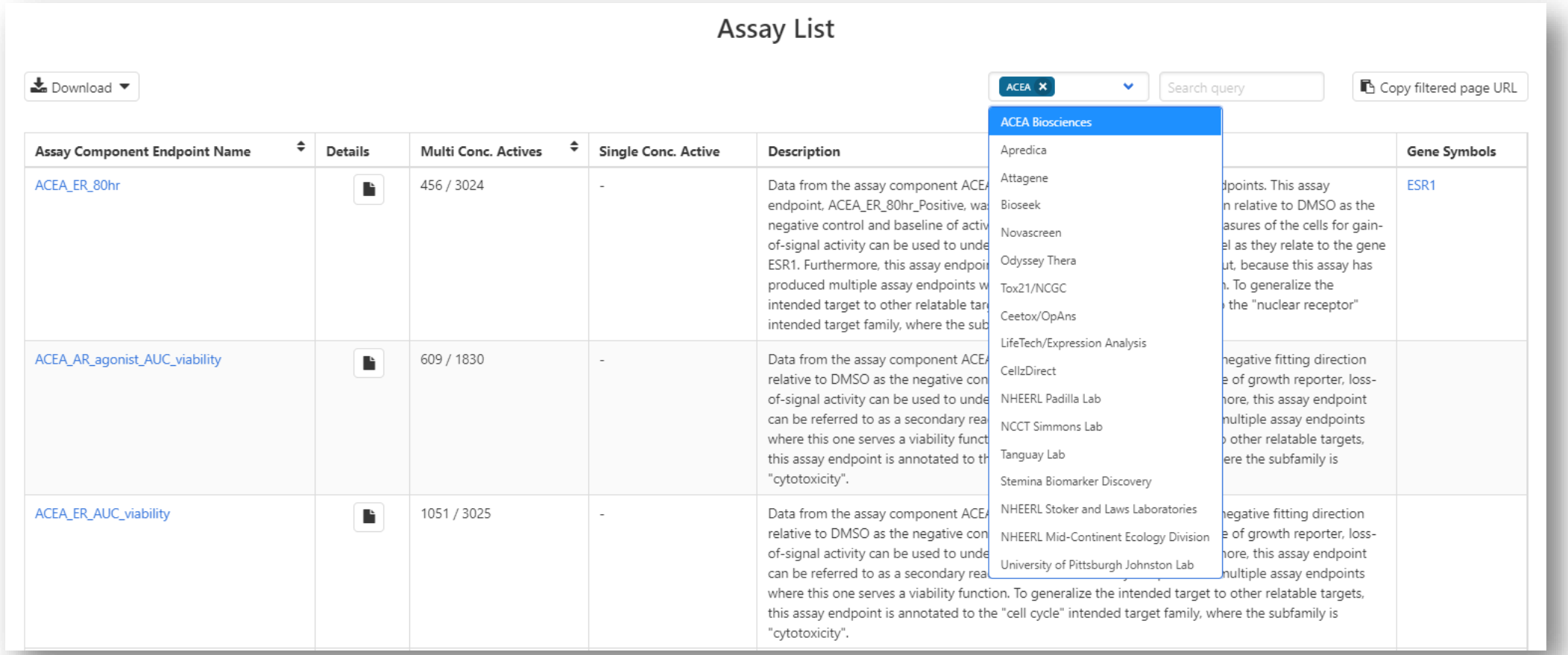
**Assay Source Description:** ACEA Biosciences, Inc. (ACEA) is a privately owned biotechnology company that developed a real-time, label-free, cell growth assay system called xCELLigence based on a microelectronic impedance readout .

**Histograms**



# Filtering by vendor….or Gene Symbol



# Use Models Derived from the Data

EPA United States Environmental Protection Agency

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

Patience Browne[*†], Richard S. Judson[‡], Warren M. Casey[§], Nicole C. Kleinstreuer[∥], and Russell S. Thomas[‡]

View Author Information

Cite this: *Environ. Sci. Technol.* 2015, 49, 14, 8804–8814
Publication Date: June 12, 2015
https://doi.org/10.1021/acs.est.5b02641



Vol. 124, No. 7 | Research

## CERAPP: Collaborative Estrogen Receptor Activity Prediction Project

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

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

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

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

View Author Information

Cite this: *Chem. Res. Toxicol.* 2017, 30, 4, 946–964
Publication Date: November 18, 2016
https://doi.org/10.1021/acs.chemrestox.6b00347

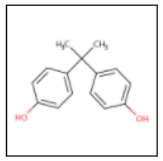

Vol. 128, No. 2 | Research

## CoMPARA: Collaborative Modeling Project for Androgen Receptor Activity

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

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

# For Endocrine (AR and ER) better to use summary models



Bisphenol A

80-05-7 | DTXSID7020182

Searched by DSSTox Substance Id.

*Positive ToxCast ER pathway agonist and ToxCast AR antagonist scores.*

- DETAILS
- EXECUTIVE SUMMARY
- PROPERTIES
- ENV. FATE/TRANSPORT
- HAZARD
- SAFETY
- ADME
- EXPOSURE
- BIOACTIVITY
  - TOXCAST: SUMMARY
  - EDSP21
  - TOXCAST/TOX21
  - PUBCHEM
  - TOXCAST: MODELS

## ToxCast: Models

ToxCast Model Predictions

Download ToxCast Model Predictions

| Model | Receptor | Agonist | Antagonist | Binding |
|---|---|---|---|---|
| ToxCast Pathway Model (AUC) | Androgen | 0.00 | 0.345 | - |
| ToxCast Pathway Model (AUC) | Estrogen | 0.450 | 0.00 | - |
| COMPARA (Consensus) | Androgen | Inactive | Active | Active |
| CERAPP Potency Level (From Literature) | Estrogen | Active (Weak) | - | Active (Weak) |
| CERAPP Potency Level (Consensus) | Estrogen | Active (Weak) | Active (Strong) | Active (Weak) |

CERAPP = consensus ER QSAR (from 17 groups)

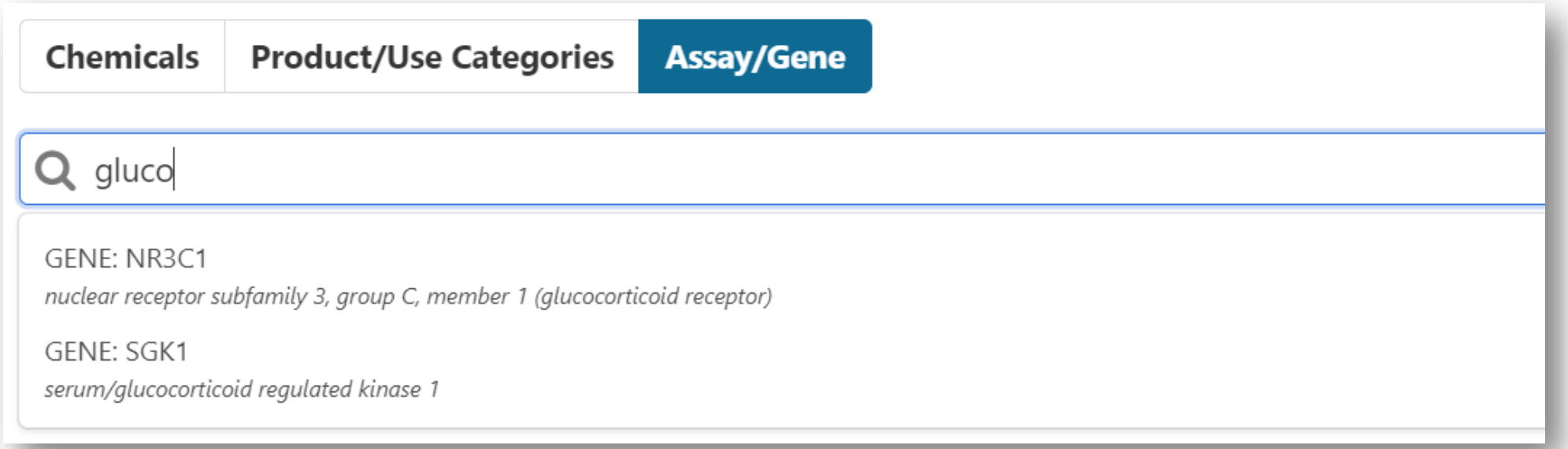
COMPARA = consensus AR QSAR

ToxCast Pathway Model AUC ER = full ER model (18 assays)

ToxCast Pathway Model AUC AR = full AR model (11 assays)

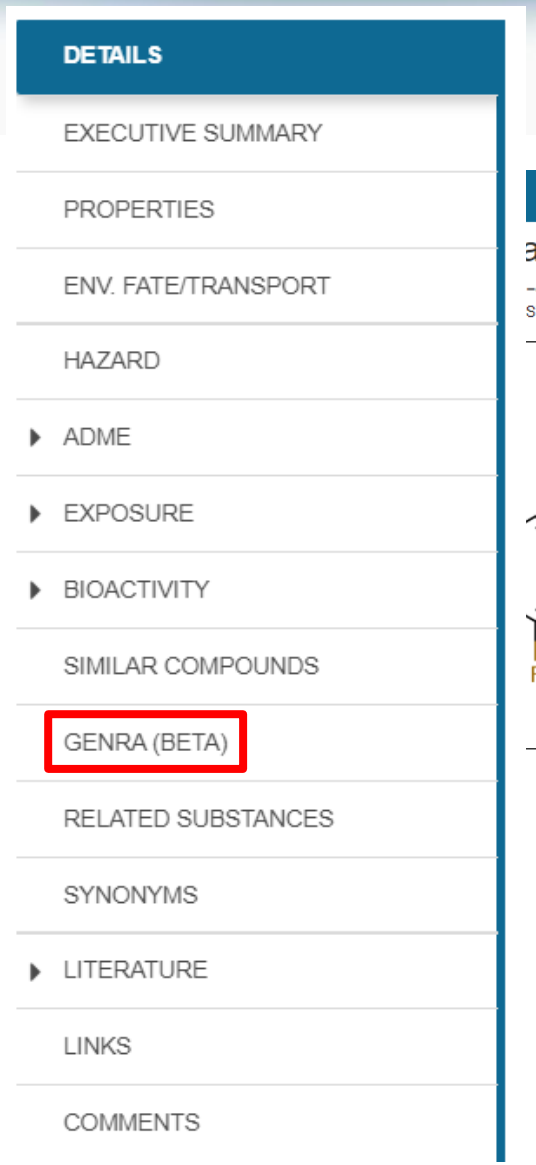
# Where do we look for assay details?

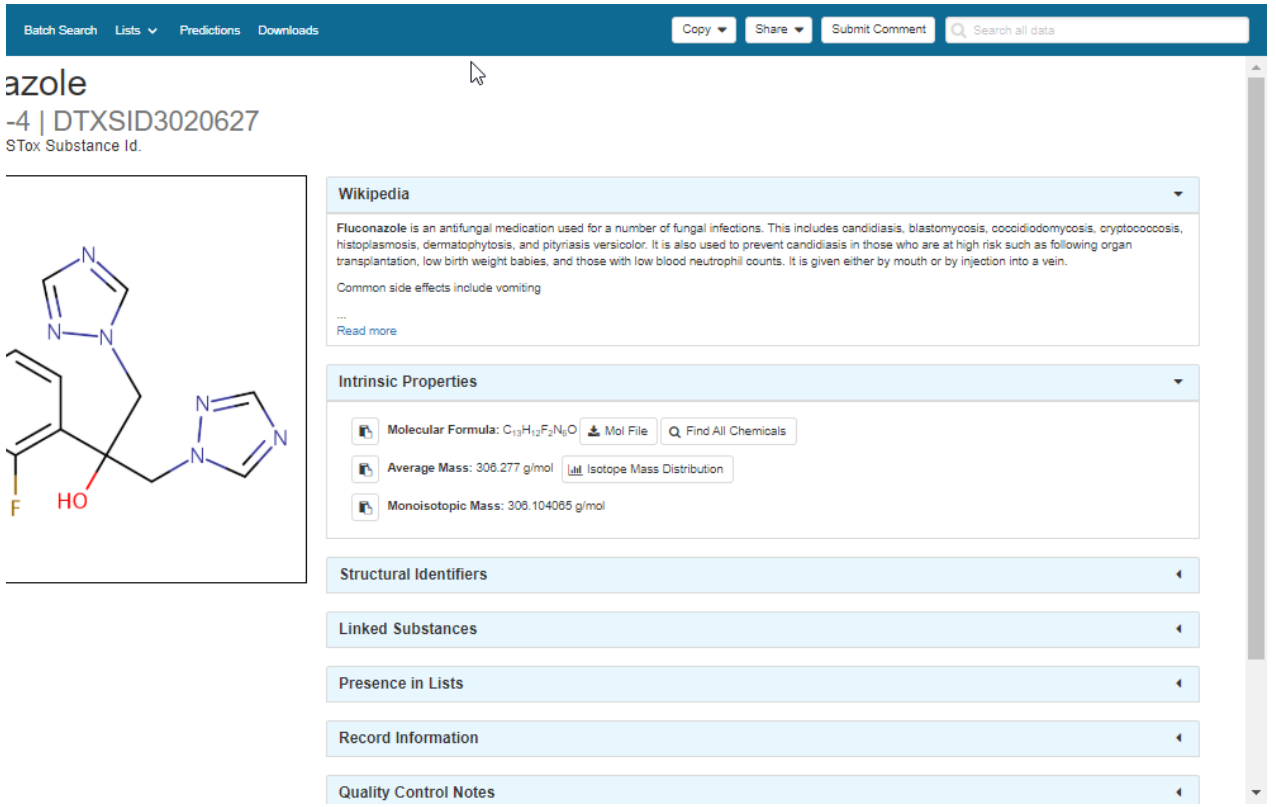
- How do we search the 100s of genes mapped against assays
- Home page: Assay/Gene Search



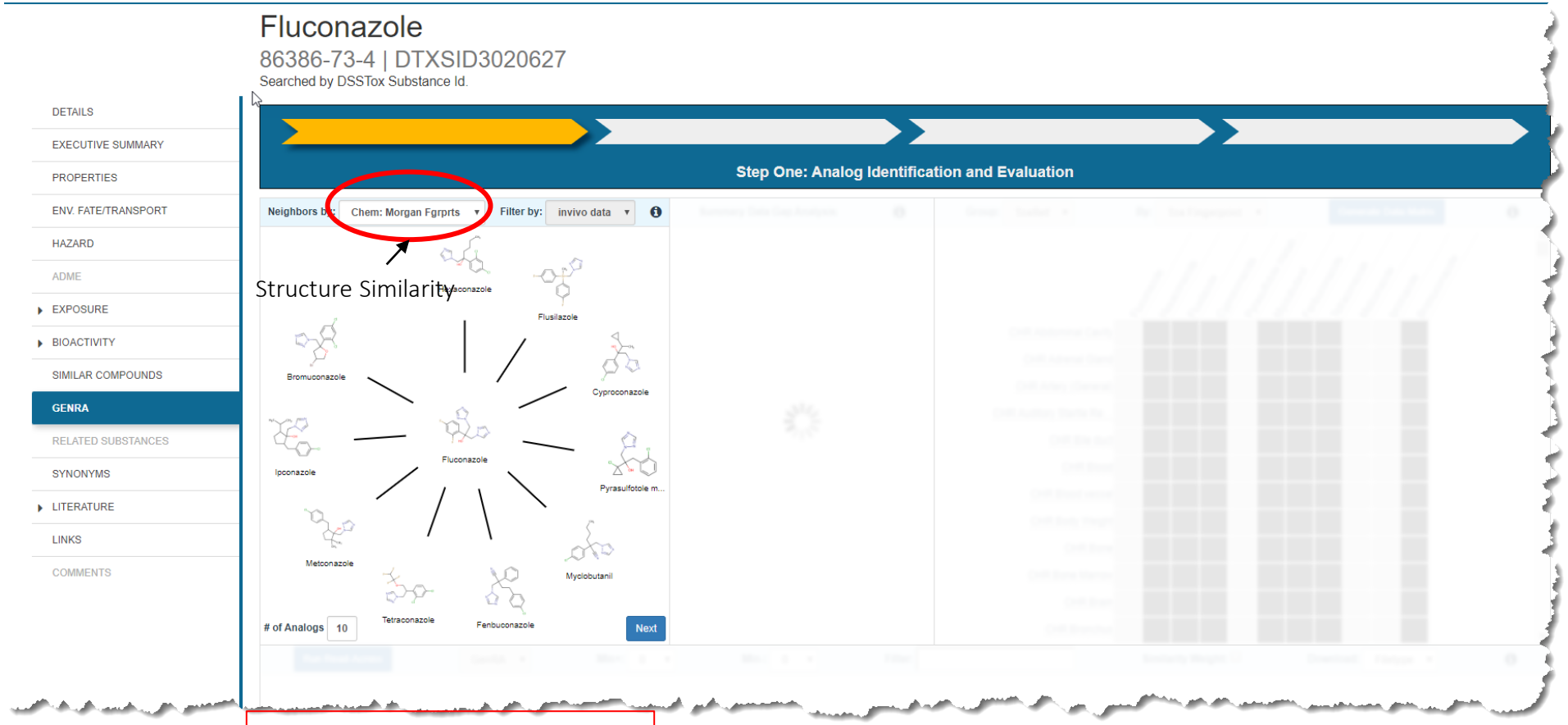
# Generalized Read-Across

# GenRA (Generalised Read-Across)



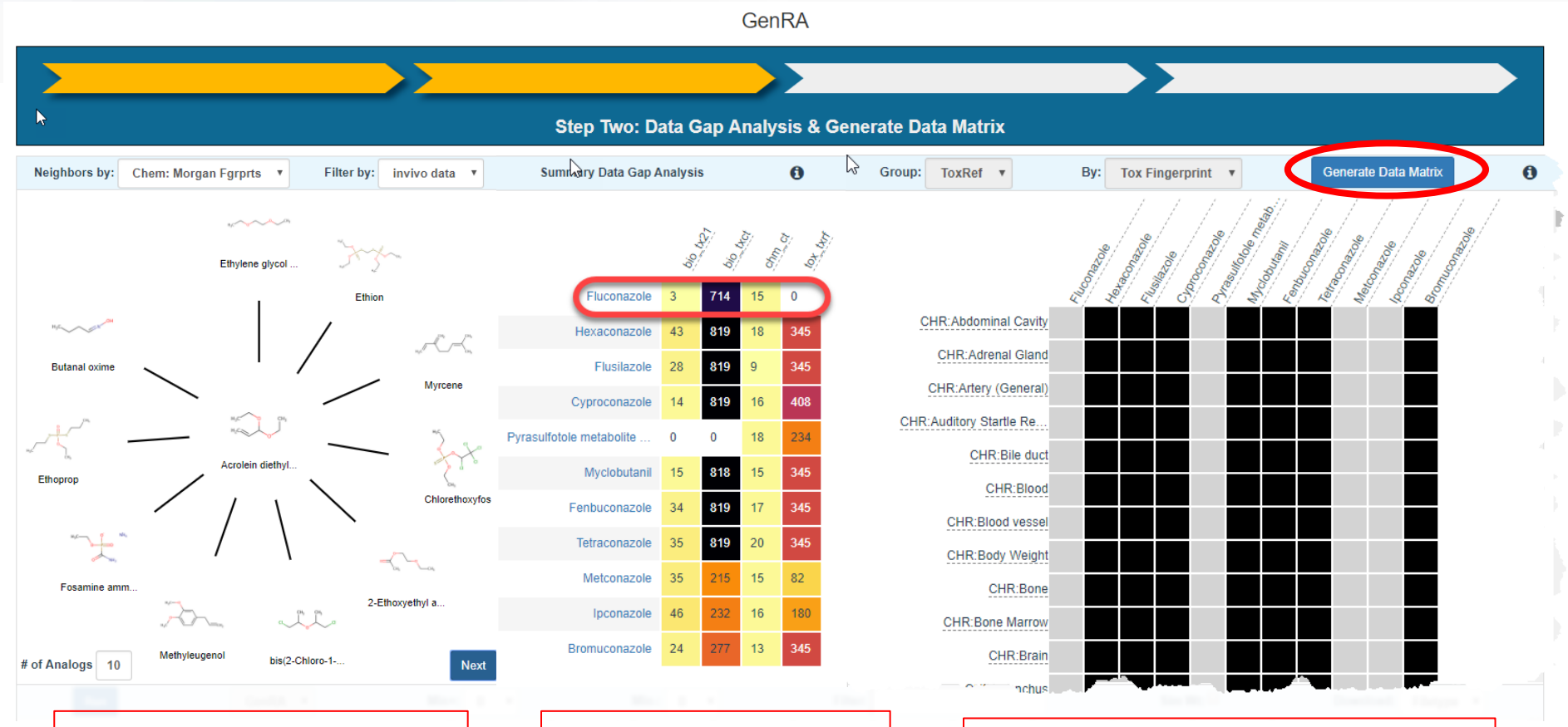



# GenRA (Generalised Read-Across)




Select and Review Analogs

# GenRA (Generalised Read-Across)

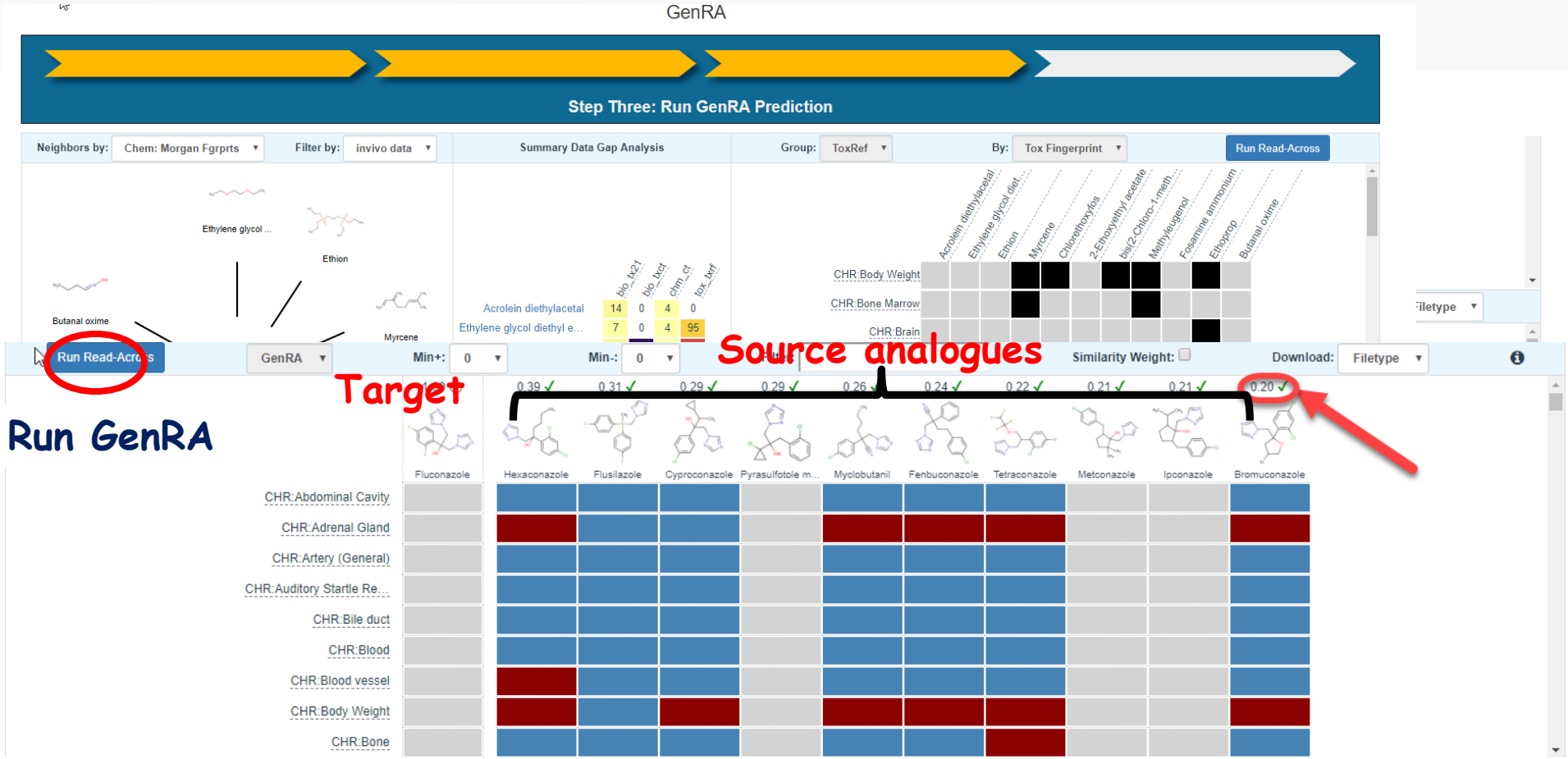



Select and Review Analogs

Review Available Data

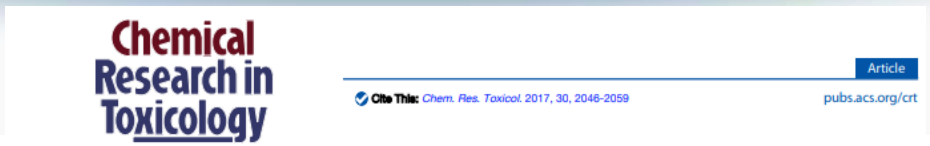
Fingerprint indicating available data

# GenRA (Generalised Read-Across)




Red : Toxicity effects.
Blue: No Toxicity effects
Grey : Absence of data

# Related Publications



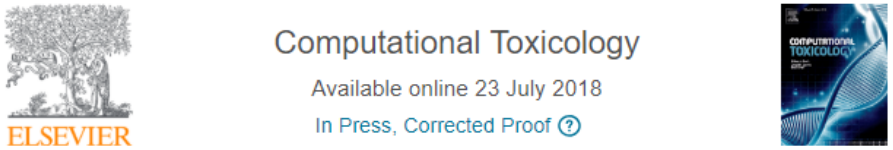

**Predicting Organ Toxicity Using *in Vitro* Bioactivity Data and Chemical Structure**

Jie Liu,[‡,§] Grace Patlewicz,[†] Antony J. Williams,[†] Russell S. Thomas,[†] and Imran Shah[*,†]

[†]National Center for Computational Toxicology, Office of Research and Development, U.S. Environmental Protection Agency, Research Triangle Park, Durham, North Carolina 27711, United States

[‡]Department of Information Science, University of Arkansas at Little Rock, Arkansas 72204, United States

[§]Oak Ridge Institute for Science Education, National Center for Computational Toxicology, Office of Research and Development, U.S. Environmental Protection Agency, Research Triangle Park, Durham, North Carolina 27711, United States




Extending the Generalised Read-Across approach (GenRA): A systematic analysis of the impact of physicochemical property information on read-across performance

George Helman [a, b], Imran Shah [b], Grace Patlewicz [b]


Systematically evaluating read-across prediction and performance using a local validity approach characterized by chemical structure and bioactivity information

Imran Shah [a], Jie Liu [b, c], Richard S. Judson [a], Russell S. Thomas [a], Grace Patlewicz [a]


Navigating through the minefield of read-across frameworks: A commentary perspective

Grace Patlewicz[a, *], Mark T.D. Cronin[b], George Helman[a, c], Jason C. Lambert[d], Lucina E. Lizarraga[d], Imran Shah[a]

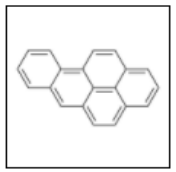
[a] National Center for Computational Toxicology (NCCT), Office of Research and Development, US Environmental Protection Agency (US EPA), 109 TW Alexander Dr, Research Triangle Park (RTP), NC 27711, USA
[b] School of Pharmacy and Biomolecular Sciences, Liverpool John Moores University, Byrom Street, Liverpool L3 3AF, UK
[c] Oak Ridge Institute for Science and Education (ORISE), 1299 Bethel Valley Road, Oak Ridge, TN 37830, USA
[d] National Center for Evaluation Assessment (NCEA), US Environmental Protection Agency (US EPA), 26 West Martin Luther King Dr, Cincinnati, OH 45268, USA

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

- We know how complex chemicals identifiers are…
  - CASRN(s)
  - Hundreds of names (maybe)
  - SMILES
  - InChIs
  - EINECS, EC numbers

- What can WE do to help you navigate the internet?

# Identifiers Support Searches in other systems



## Benzo(a)pyrene

50-32-8 | DTXSID2020139

Searched by DSSTox Substance Id.

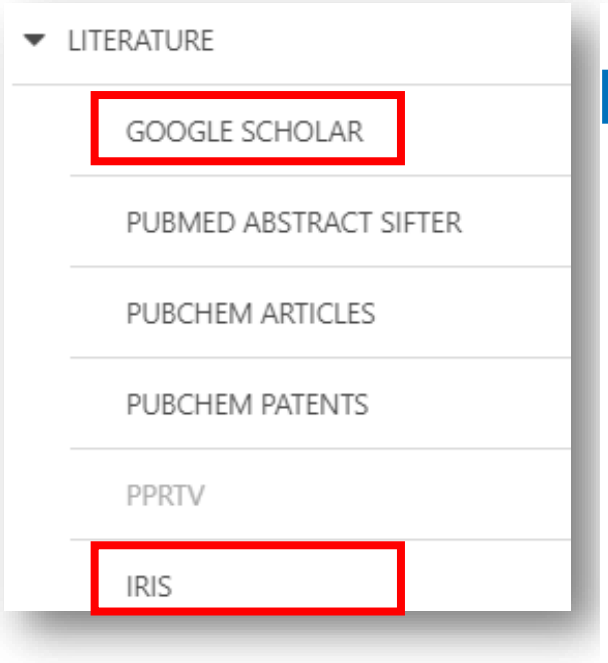
### Synonyms

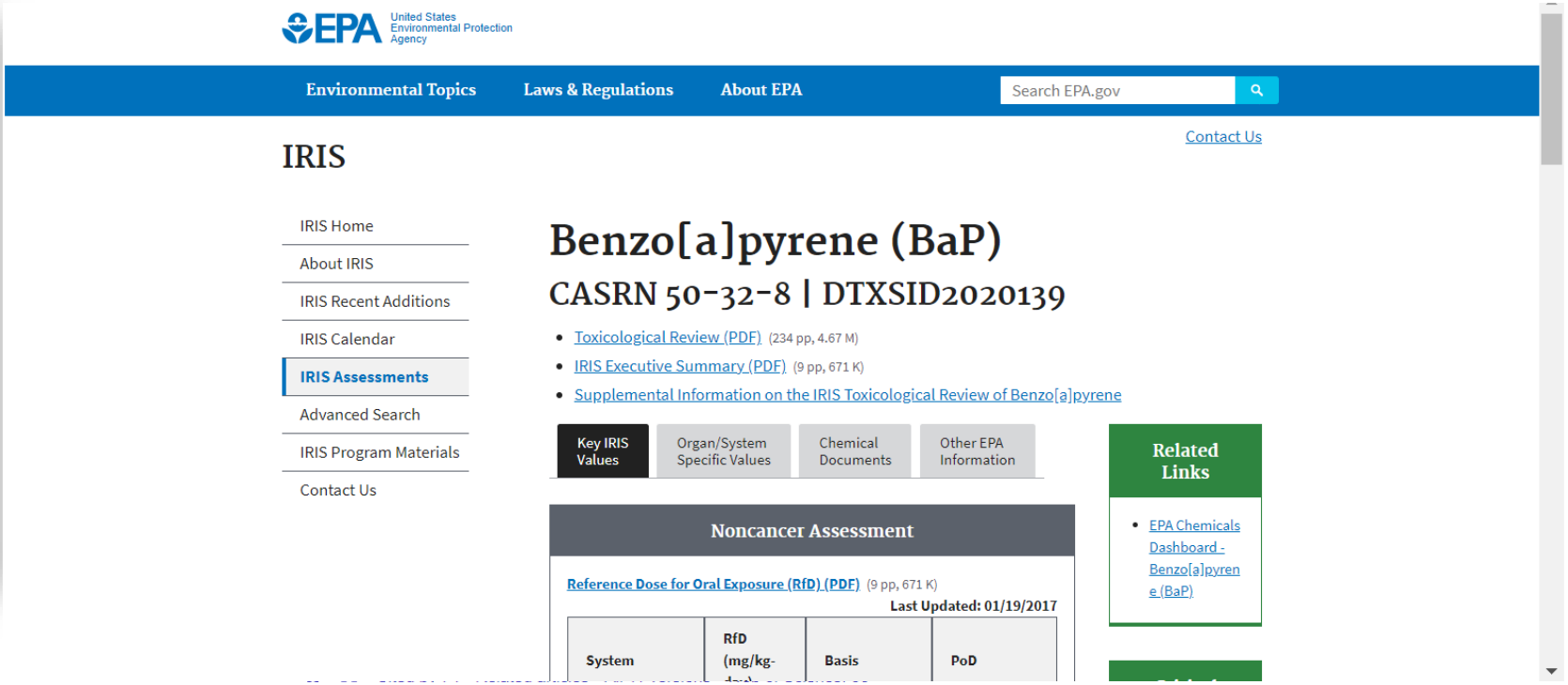
Download 25 Search query

| Synonym | Quality |
|---|---|
| **Benzo(a)pyrene** | **Valid** |
| **Benzo[pqr]tetraphene** | **Valid** |
| **Benzo[a]pyrene** | **Valid** |
| **50-32-8** Active CAS-RN | **Valid** |
| **BaP** | **Valid** |
| *Benzo[a]pyrene* | *Good* |
| *3,4-Benz[a]pyrene* | *Good* |
| *3,4-Benzopyrene* | *Good* |
| *3,4-Benzpyrene* | *Good* |
| *6,7-Benzopyrene* | *Good* |
| *BENZ(A)PYREN* | *Good* |
| *Benz(a)pyrene* | *Good* |
| *Benz[a]pyrene* | *Good* |

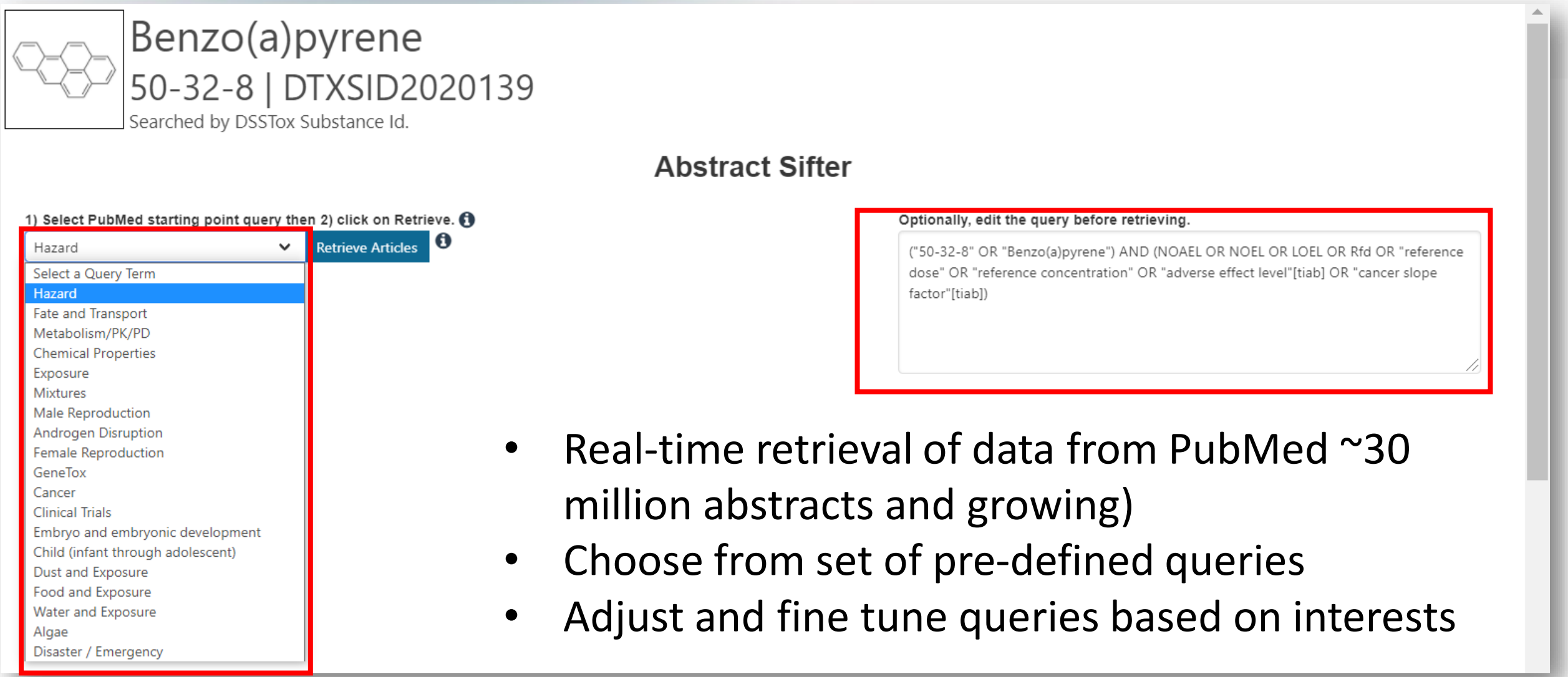
# Identifiers are used in the app

- Identifiers are used to feed and link into “Literature”



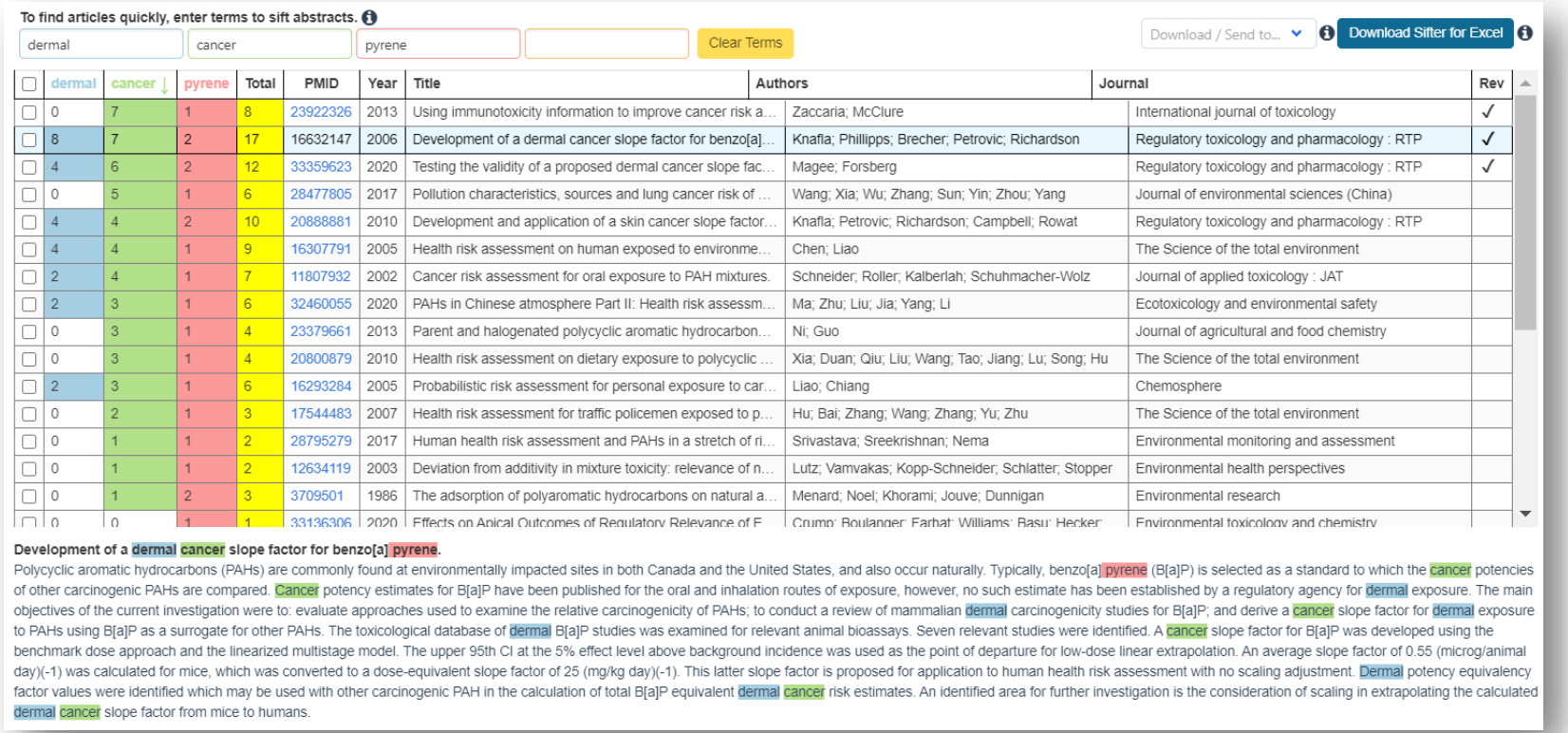
# Literature Searching




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

# Literature Searching

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



To find articles quickly, enter terms to sift abstracts.

dermal | cancer | pyrene | Clear Terms | Download / Send to... | Download Sifter for Excel

| dermal | cancer | pyrene | Total | PMID | Year | Title | Authors | Journal | Rev |
|---|---|---|---|---|---|---|---|---|---|
| 0 | 7 | 1 | 8 | 23922326 | 2013 | Using immunotoxicity information to improve cancer risk a… | Zaccaria; McClure | International journal of toxicology | ✓ |
| 8 | 7 | 2 | 17 | 16632147 | 2006 | Development of a dermal cancer slope factor for benzo[a]… | Knafla; Phillipps; Brecher; Petrovic; Richardson | Regulatory toxicology and pharmacology : RTP | ✓ |
| 4 | 6 | 2 | 12 | 33359623 | 2020 | Testing the validity of a proposed dermal cancer slope fac… | Magee; Forsberg | Regulatory toxicology and pharmacology : RTP | ✓ |
| 0 | 5 | 1 | 6 | 28477805 | 2017 | Pollution characteristics, sources and lung cancer risk of … | Wang; Xia; Wu; Zhang; Sun; Yin; Zhou; Yang | Journal of environmental sciences (China) | |
| 4 | 4 | 2 | 10 | 20888881 | 2010 | Development and application of a skin cancer slope factor… | Knafla; Petrovic; Richardson; Campbell; Rowat | Regulatory toxicology and pharmacology : RTP | |
| 4 | 4 | 1 | 9 | 16307791 | 2005 | Health risk assessment on human exposed to environme… | Chen; Liao | The Science of the total environment | |
| 2 | 4 | 1 | 7 | 11807932 | 2002 | Cancer risk assessment for oral exposure to PAH mixtures. | Schneider; Roller; Kalberlah; Schuhmacher-Wolz | Journal of applied toxicology : JAT | |
| 2 | 3 | 1 | 6 | 32460055 | 2020 | PAHs in Chinese atmosphere Part II: Health risk assessm… | Ma; Zhu; Liu; Jia; Yang; Li | Ecotoxicology and environmental safety | |
| 0 | 3 | 1 | 4 | 23379661 | 2013 | Parent and halogenated polycyclic aromatic hydrocarbon… | Ni; Guo | Journal of agricultural and food chemistry | |
| 0 | 3 | 1 | 4 | 20800879 | 2010 | Health risk assessment on dietary exposure to polycyclic … | Xia; Duan; Qiu; Liu; Wang; Tao; Jiang; Lu; Song; Hu | The Science of the total environment | |
| 2 | 3 | 1 | 6 | 16293284 | 2005 | Probabilistic risk assessment for personal exposure to car… | Liao; Chiang | Chemosphere | |
| 0 | 2 | 1 | 3 | 17544483 | 2007 | Health risk assessment for traffic policemen exposed to p… | Hu; Bai; Zhang; Wang; Zhang; Yu; Zhu | The Science of the total environment | |
| 0 | 1 | 1 | 2 | 28795279 | 2017 | Human health risk assessment and PAHs in a stretch of ri… | Srivastava; Sreekrishnan; Nema | Environmental monitoring and assessment | |
| 0 | 1 | 1 | 2 | 12634119 | 2003 | Deviation from additivity in mixture toxicity: relevance of n… | Lutz; Vamvakas; Kopp-Schneider; Schlatter; Stopper | Environmental health perspectives | |
| 0 | 1 | 2 | 3 | 3709501 | 1986 | The adsorption of polyaromatic hydrocarbons on natural a… | Menard; Noel; Khorami; Jouve; Dunnigan | Environmental research | |
| 0 | 0 | 1 | 1 | 33136306 | 2020 | Effects on Apical Outcomes of Regulatory Relevance of E… | Crump; Boulanger; Farhat; Williams; Basu; Hecker | Environmental toxicology and chemistry | |

**Development of a dermal cancer slope factor for benzo[a] pyrene.**

Polycyclic aromatic hydrocarbons (PAHs) are commonly found at environmentally impacted sites in both Canada and the United States, and also occur naturally. Typically, benzo[a] pyrene (B[a]P) is selected as a standard to which the cancer potencies of other carcinogenic PAHs are compared. Cancer potency estimates for B[a]P have been published for the oral and inhalation routes of exposure, however, no such estimate has been established by a regulatory agency for dermal exposure. The main objectives of the current investigation were to: evaluate approaches used to examine the relative carcinogenicity of PAHs; to conduct a review of mammalian dermal carcinogenicity studies for B[a]P; and derive a cancer slope factor for dermal exposure to PAHs using B[a]P as a surrogate for other PAHs. The toxicological database of dermal B[a]P studies was examined for relevant animal bioassays. Seven relevant studies were identified. A cancer slope factor for B[a]P was developed using the benchmark dose approach and the linearized multistage model. The upper 95th CI at the 5% effect level above background incidence was used as the point of departure for low-dose linear extrapolation. An average slope factor of 0.55 (microg/animal day)(-1) was calculated for mice, which was converted to a dose-equivalent slope factor of 25 (mg/kg day)(-1). This latter slope factor is proposed for application to human health risk assessment with no scaling adjustment. Dermal potency equivalency factor values were identified which may be used with other carcinogenic PAH in the calculation of total B[a]P equivalent dermal cancer risk estimates. An identified area for further investigation is the consideration of scaling in extrapolating the calculated dermal cancer slope factor from mice to humans.

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

## Benzo(a)pyrene

50-32-8 | DTXSID2020139

Searched by DSSTox Substance Id.

### General

- EPA Substance Registry Service
- PubChem
- Chemspider
- CPCat
- DrugBank
- Wikipedia
- MSDS Lookup
- ChEMBL
- ToxPlanet
- ACS Reagent Chemicals
- Wolfram Alpha
- ECHA Infocard
- ChemAgora
- Consumer Product Information Database
- ChEBI
- NIST Chemistry Webbook
- WEBWISER
- PubChem Safety Sheet
- Consumer Product Information Database
- PubChem: Chemical Vendors

### Toxicology

- ACToR
- DrugPortal
- CCRIS
- ChemView
- CTD
- eChemPortal
- Gene-Tox
- HSDB
- ACToR PDF Report
- CREST
- National Air Toxics Assessment
- ECOTOX
- ChemView
- Chemical Checker
- BindingDB
- CalEPA OEHHA
- NIOSH IDLH Values
- LactMed
- ECOTOX

### Publications

- Toxline
- PPRTVWEB
- PubMed
- IRIS Assessments
- EPA HERO
- NIOSH Skin Notation Profiles
- NIOSH Pocket Guide
- RSC Publications
- BioCaddie DataMed
- Springer Materials
- Bielefeld Academic Search Engine
- CORE Literature Search
- Google Books (Text Search)
- Google Patents (Text search)
- Google Scholar (Text search)
- Google Patents (Structure search)
- Google Books (Structure Search)
- Google Scholar (Structure search)
- Federal Register

### Analytical

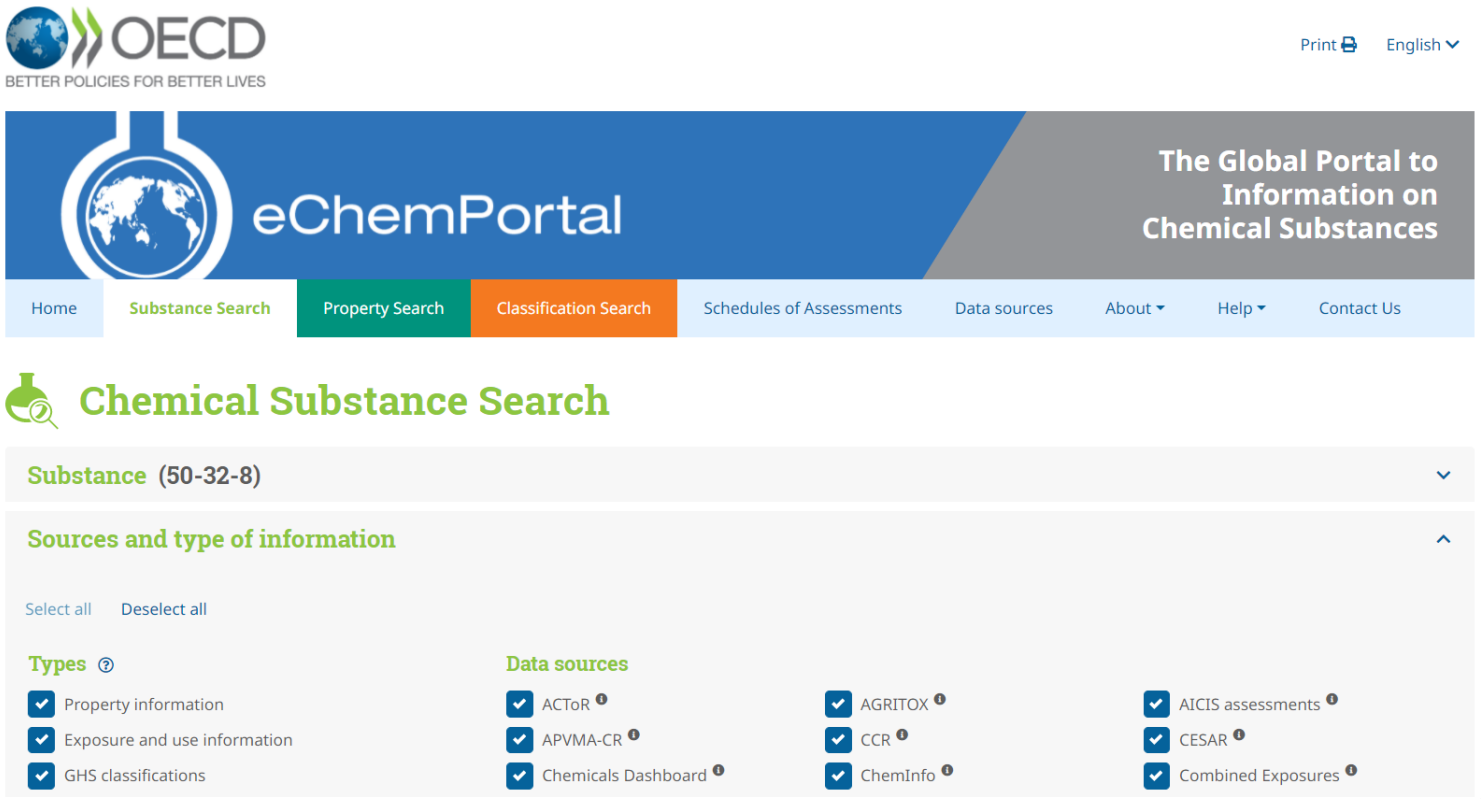
- RSC Analytical Abstracts
- Tox21 Analytical Data
- MONA: MassBank North America
- mzCloud
- NIST IR Spectrum
- NIST MS Spectrum
- MassBank
- NIST Antoine Constants
- IR Spectra on PubChem
- NIST Kovats Index values
- Protein DataBank
- National Environmental Methods Index

### Prediction

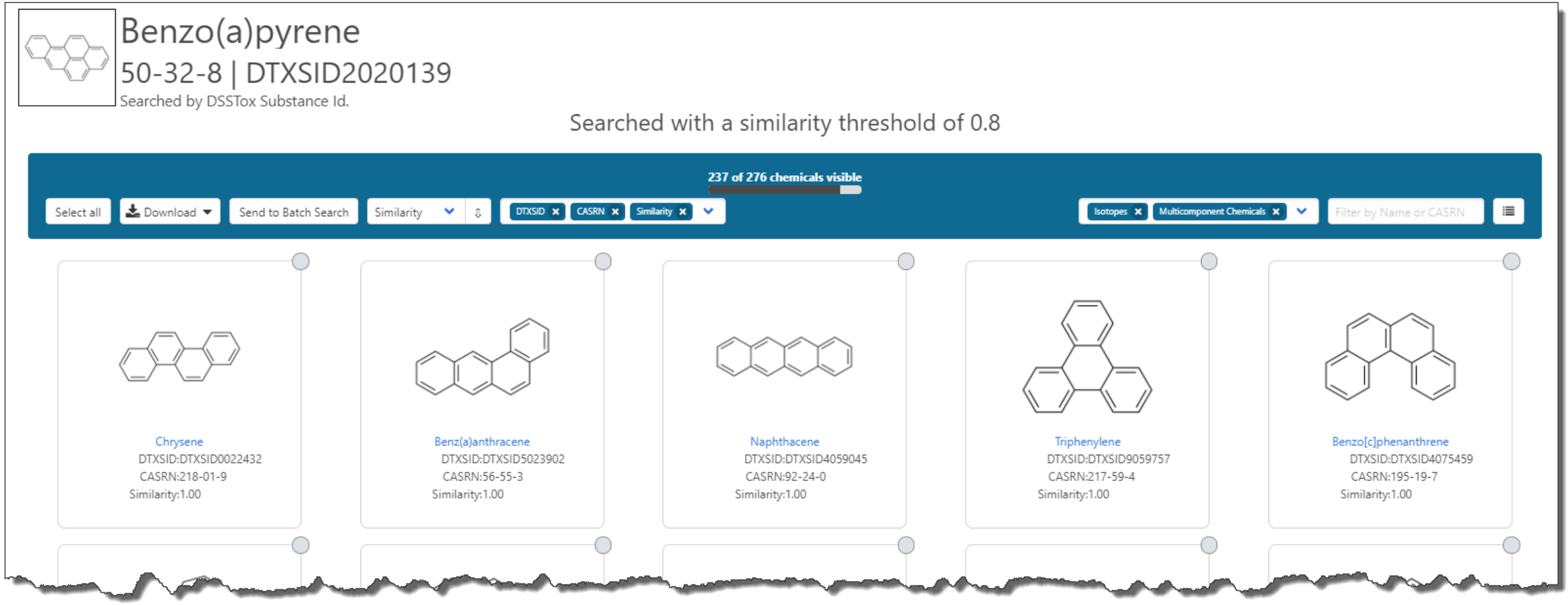
- 2D NMR HSQC/HMBC Prediction
- Carbon-13 NMR Prediction
- Proton NMR Prediction
- ChemRTP Predictor
- LSERD

# External Links

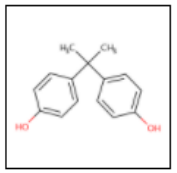
- Links to ~90 websites providing access to additional data on the chemical of interest

# Similarity Searching



# Related Substances



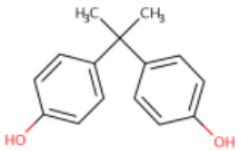
## Bisphenol A

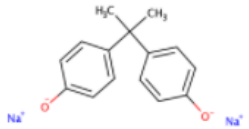
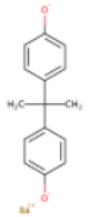
80-05-7 | DTXSID7020182

Searched by DSSTox Substance Id.

9 chemicals

Select all | Download | Send to Batch Search | Relationship | DTXSID × | CASRN × | TOXCAST × | Hide chemicals that are: | Filter by Name or CASRN

| Searched Chemical | Polymer | Polymer | Polymer | Predecessor: Component |
|---|---|---|---|---|
|  | 2 related chemical structures with this substance | 2 related chemical structures with this substance | 3 related chemical structures with this substance | 4 related chemical structures with this substance |
| Bisphenol A<br>DTXSID:DTXSID7020182<br>CASRN:80-05-7<br>TOXCAST:217/1152 | Formaldehyde, polymer with bisphenol A<br>DTXSID:DTXSID3049627<br>CASRN:25085-75-0<br>TOXCAST:- | Bisphenol A/ Epichlorohydrin resin<br>DTXSID:DTXSID0050479<br>CASRN:25068-38-6<br>TOXCAST:- | Bisphenol A-epichlorohydrin-polyformal...<br>DTXSID:DTXSID9050480<br>CASRN:28906-96-9<br>TOXCAST:- | Fatty acids, C18-unsatd., dimers, polyme...<br>DTXSID:DTXSID40105886<br>CASRN:106906-26-7<br>TOXCAST:- |

| Predecessor: Component | Predecessor: Component | Salt Form | Salt Form |
|---|---|---|---|
| 3 related chemical structures with this substance | 2 related chemical structures with this substance |  |  |
| ...rohydrin-2,2',6,6'-tet... | Phenoxy Resin | Disodium 4,4'-isopropylidenediphenolate | Barium(2+) 4,4'-isopropylidenebispheno... |

...anced_search/index

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Environmental Protection
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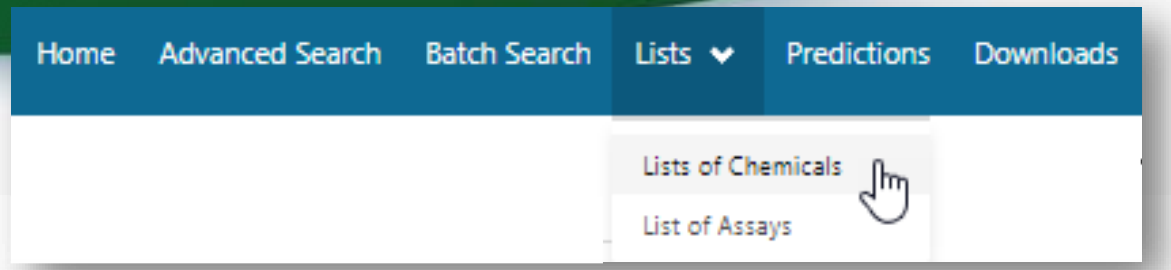
# Chemical Lists and Categories

# Example: AEGLs list




## AEGLS: Acute Exposure Guideline Levels

Search AEGLVALUES Chemicals

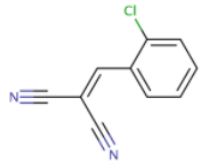
Identifier substring search

**List Details**

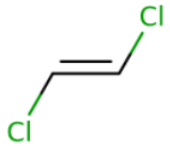
**Description:** Acute Exposure Guideline Level (AEGLs) values are intended to protect most individuals in the general population, including those that might be particularly susceptible to the harmful effects of the chemicals. Acute exposure guideline levels (AEGLs) describe the human health effects from once-in-a-lifetime, or rare, exposure to airborne chemicals. Used by emergency responders when dealing with chemical spills or other catastrophic exposures, AEGLs are set through a collaborative effort of the public and private sectors worldwide.
**Number of Chemicals:** 174

174 chemicals

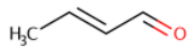
Select all | Download | Send to Batch Search | Name | CASRN | DTXSID | Hide chemicals that are: | Filter by Name or CASRN



(2-Chlorobenzylidene)propanedinitrile
CASRN:2698-41-1
DTXSID:DTXSID9020297



(E)-1,2-Dichloroethylene
CASRN:156-60-5
DTXSID:DTXSID7024031



(E)-Crotonaldehyde
CASRN:123-73-9
DTXSID:DTXSID6020351

(Z)-1,2-Dichloroethylene
CASRN:156-59-2
DTXSID:DTXSID2024030

# PFAS lists of Chemicals

United States Environmental Protection Agency

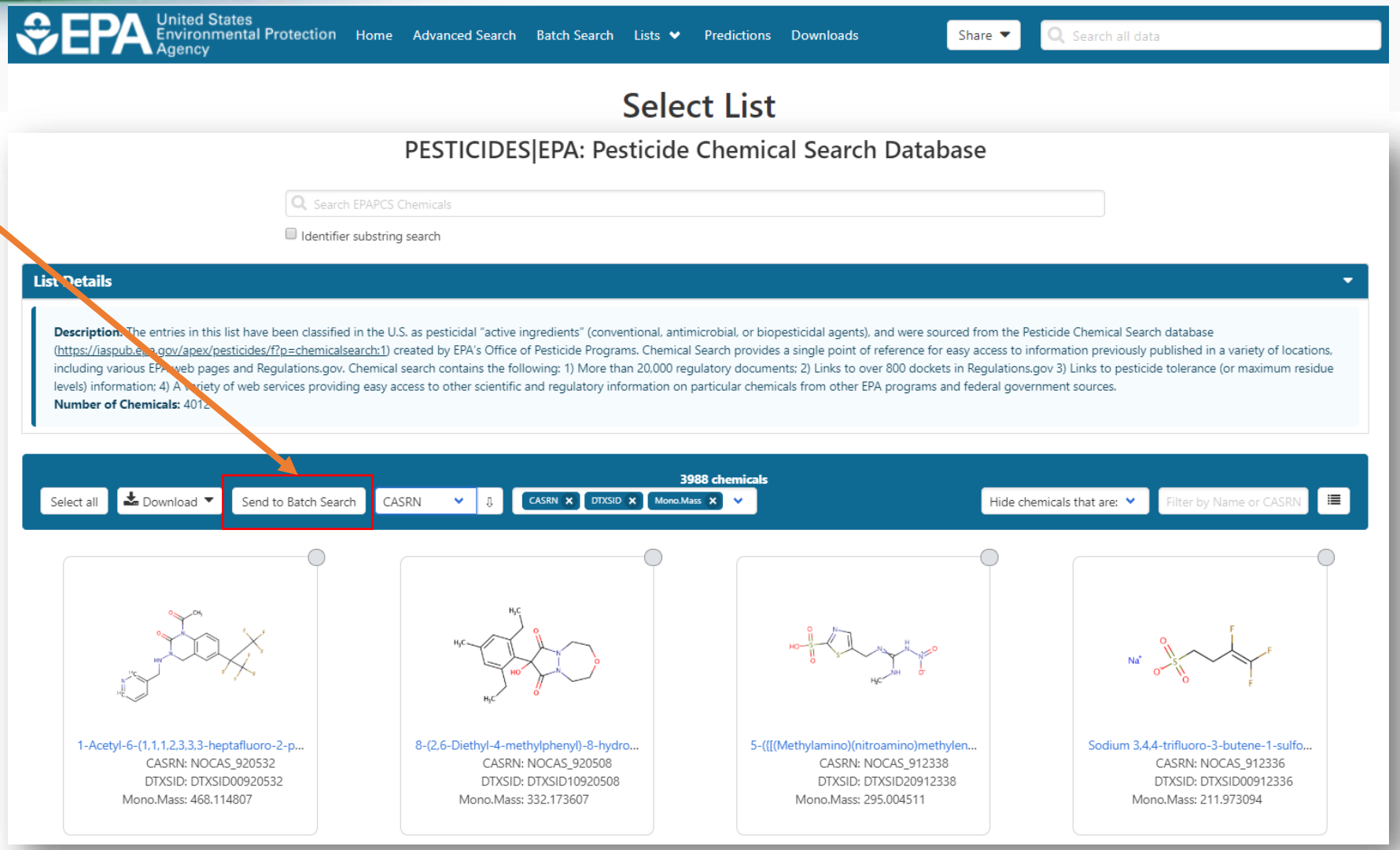
## Select List

Download | Columns | PFAS | Copy Filtered Lists URL

| List Acronym | List Name | Last Updated | Number of Chemicals | List Description |
|---|---|---|---|---|
| EPAPFAS75S1 | PFAS\|EPA: 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. |
| EPAPFAS75S2 | PFAS\|EPA: List of 75 Test Samples (Set 2) | 2019-02-21 | 75 | PFAS list corresponds to a second set of 75 samples (Set 2) submitted for testing screens conducted by EPA researchers in collaboration with researchers at the National Toxicology Program. |
| EPAPFASCAT | PFAS\|EPA Structure-based 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\|EPA: 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\|EPA: ToxCast Chemical Inventory | 2018-06-29 | 430 | PFAS chemicals included in EPA's expanded ToxCast chemical inventory and available for testing. |
| EPAPFASRL | PFAS\|EPA: Cross-Agency Research List | 2017-11-16 | 199 | 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. |
| PFASKEMI | PFAS: List from the Swedish Chemicals Agency (KEMI) Report | 2017-02-09 | 2416 | 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. |
| PFASOECD | PFAS: Listed in OECD Global Database | 2018-05-16 | 4729 | OECD released a New Comprehensive Global Database of Per- and Polyfluoroalkyl Substances, (PFASs) listing more than 4700 new PFAS |
| PFASTRIER | PFAS Community-Compiled List (Trier et al., 2015) | 2017-07-16 | 597 | PFASTRIER community-compiled public listing of PFAS (Trier et al, 2015) |

# Curated List of Pesticides

- Find list of interest
- Select list and send to batch



EPA
United States
Environmental Protection
Agency

# Batch Searching

# Batch Searching

- Singleton searches are great but…
- …we generally want data on LOTS of chemicals!

- Typical questions
  - What are the structures for a set of chemical names? Set of CASRNs?
  - Can I get chemical lists in Excel files? As a list of SMILES strings? Can I get an SDF file?
  - Can I include predicted properties? OPERA? TEST?
  - Are “these chemicals” screened in Toxcast?
  - I need masses and formulae for a list of chemicals

# Access data *en masse* for thousands of chemicals…

EPA United States Environmental Protection Agency

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

## Batch Search

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

### Step Three: Select Download Data or Display Chemicals

Please enter one identifier per line

**Select Input Type(s)**

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

**Enter Identifiers to Search** (One per line. Searches should be limited to <5000 identifiers.)

Sodium azide
O,O-Dimethyl S-[(4-oxo-1,2,3-benzotriazin-3(4H)-yl)methyl] phosphorodithioate
(Trichloromethyl)benzene
100-44-7
(Chloromethyl)benzene
98-07-7
111-44-4
1-Chloro-2-(2-chloroethoxy)ethane
Chloro(chloromethoxy)methane
2-(Butan-2-yl)-4,6-dinitrophenol

Display All Chemicals | Download Chemical Data

# Select Output Format and Content

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

**Select Output Format:**

Excel

Download

**Customize Results**

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

**Chemical Identifiers**

- [x] DTXSID
- [x] Chemical Name
- [ ] DTXCID
- [ ] 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

**Metadata**

- [ ] Curation Level Details
- [ ] NHANES/Predicted Exposure
- [ ] Data Sources
- [ ] Include ToxVal Data Availability
- [ ] Assay Hit Count
- [ ] Number of PubMed Articles
- [ ] PubChem Data Sources
- [ ] CPDat Product Occurrence Count
- [ ] IRIS
- [ ] PPRTV
- [ ] Wikipedia Article
- [ ] QC Notes
- [ ] Include links to ACToR reports - SLOW! (BETA)

**Presence in Lists:**

- [ ] 40CFR116.4 Designation of Hazardous Substances (Above Ground Storage Tanks)
- [ ] 40CFR355 Extremely Hazardous Substance List and Threshold Planning Quantities
- [ ] AEGLS: Acute Exposure Guideline Levels
- [ ] ANDROGEN: Androgen Receptor Chemicals
- [ ] ARTICLE; Bench-Mark Dose Human Health Assessment List (Wignall et al., 2014)
- [ ] ARTICLE: Collaborative Estrogen Receptor Activity Prediction Project (CERAPP)
- [ ] ARTICLE: Collaborative Estrogen Receptor Activity Prediction Project (COMPARA)
- [ ] ATSDR Toxicological Profiles
- [ ] ATSDR: Minimal Risk Levels (MRLs) for Hazardous Substances
- [ ] ATSDR: Toxic Substances Portal Chemical List
- [ ] California Office of Environmental Health Hazard Assessment
- [ ] Canadian Domestic Substances List 2019
- [ ] CATEGORY: Amino acids
- [ ] CATEGORY: Color Index dyes
- [ ] CATEGORY: Flame Retardants

# Batch Search CASRNs

EPA United States Environmental Protection Agency

## Batch Search

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

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

Please enter one identifier per line

**Chemical Identifiers**
- [x] DTXSID
- [x] Chemical Name
- [ ] DTXCID
- [x] CAS-RN
- [x] InChIKey
- [x] IUPAC Name

**Structures**
- [ ] Mol File
- [ ] SMILES
- [ ] InChI String
- [x] MS-Ready SMILES
- [ ] QSAR-Ready SMILES

**Intrinsic And Predicted Properties**
- [x] Molecular Formula
- [ ] Average Mass
- [ ] Monoisotopic Mass
- [ ] TEST Model Predictions
- [x] OPERA Model Predictions

**Metadata**
- [ ] Curation Level Details
- [ ] NHANES/Predicted Exposure
- [ ] Data Sources
- [x] Include ToxVal Data Availability
- [x] Assay Hit Count
- [x] Number of PubMed Articles

| | A | B | C | D | E | F | G | H | I | J | K | L | M | N | O | P | Q |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | INPUT | FOUND_BY | DTXSID | PREFERRE | CASRN | INCHIKEY | IUPAC_NAI | MOLECULA | TOXVAL_D | TOXCAST_ | TOXCAST_ | MS_READY | NUMBER_C | IRIS_LINK | PPRTV_LIN | ATMOSPHE | BIOCONCE |
| 2 | 534-52-1 | CAS-RN | DTXSID10 | 2-Methyl-4,6 | 534-52-1 | ZXVONLUN | 2-Methyl-4,6 | C7H6N2O5 | Y | 27.56 | 261/947 | CC1=C(O)C | 179 | - | Y | 1.571E-12 | 2.88959 |
| 3 | 115-21-9 | CAS-RN | DTXSID70 | Ethyl silicon | 115-21-9 | ZOYFEXPF | Trichloro(eth | C2H5Cl3Si | Y | - | - | - | - | - | - | 8.289E-12 | 13.9658 |
| 4 | 111-44-4 | CAS-RN | DTXSID90 | Bis(2-chloro | 111-44-4 | ZNSMNVML | 1-Chloro-2-( | C4H8Cl2O | Y | 1.12 | 10/891 | ClCCOCCCl | 12 | Y | - | 2.647E-12 | 9.99608 |
| 5 | 2763-96-4 | CAS-RN | DTXSID50 | Muscimol | 2763-96-4 | ZJQHPWUV | 5-(Aminome | C4H6N2O2 | Y | - | - | NCC1=CC(( | 4308 | - | - | 1.179E-10 | 5.05695 |
| 6 | 1464-53-5 | CAS-RN | DTXSID00 | 2,2'-Bioxiran | 1464-53-5 | ZFIVKAOQE | 2,2'-Bioxiran | C4H6O2 | Y | - | - | C1OC1C1C | 363 | - | - | 4.383E-12 | 1.27107 |
| 7 | 22224-92-6 | CAS-RN | DTXSID30 | Fenamiphos | 22224-92- | ZCJPOPBZI | Ethyl 3-meth | C13H22NO3 | Y | 10.8 | 105/972 | CCOP(=O)( | 58 | Y | - | 1.66E-11 | 2.3394 |
| 8 | 359-06-8 | CAS-RN | DTXSID40 | Fluoroacetyl | 359-06-8 | ZBHDTYQJ | Fluoroacetyl | C2H2ClFO | Y | - | - | FCC(Cl)=O | - | - | - | 3.513E-13 | 4.49379 |
| 9 | 5344-82-1 | CAS-RN | DTXSID40 | 1-(o-Chloroj | 5344-82-1 | YZUKKTCD | N-(2-Chloroj | C7H7ClN2S | Y | - | - | NC(=S)NC1 | - | - | - | 2.482E-11 | 9.95206 |
| 10 | 7446-18-6 | CAS-RN | DTXSID10 | Thallium (I) s | 7446-18-6 | YTQVHRVI | Dithallium(1- | O4STl2 | Y | - | - | - | 34 | Y | Y | - | - |
| 11 | 62207-76-5 | CAS-RN | DTXSID40 | Bis(3-fluoros | 62207-76- | YRZXYIHD | - | C16H14CoF | Y | - | - | - | - | - | - | - | - |
| 12 | 66-81-9 | CAS-RN | DTXSID60 | Cycloheximi | 66-81-9 | YPHMISFO | 4-{(2R)-2-[(3 | C15H23NO4 | Y | 32.27 | 294/911 | CC1CC(C)C | 18709 | - | - | 1.756E-11 | 2.81761 |
| 13 | 106-96-7 | CAS-RN | DTXSID30 | Propargyl br | 106-96-7 | YORCIIVHU | 3-Bromopro | C3H3Br | Y | - | - | BrCC#C | - | - | - | 1.069E-11 | 10.4968 |
| 14 | 315-18-4 | CAS-RN | DTXSID70 | Mexacarbat | 315-18-4 | YNEVBPNZ | 4-(Dimethyla | C12H18N2C | Y | 5.11 | 12/235 | CNC(=O)OC | 27 | - | - | 1.447E-11 | 26.2914 |
| 15 | 110-00-9 | CAS-RN | DTXSID60 | Furan | 110-00-9 | YLQBMQCU | Furan | C4H4O | Y | 0.0 | 0/235 | O1C=CC=C | 919 | Y | - | 4.019E-11 | 5.01648 |
| 16 | 3037-72-7 | CAS-RN | DTXSID20 | 4-(diethoxyn | 3037-72-7 | YHFFINXFN | 4-[Diethoxy( | C9H23NO2S | Y | - | - | - | - | - | - | 5.95E-12 | 6.71292 |
| 17 | 75-44-5 | CAS-RN | DTXSID00 | Phosgene | 75-44-5 | YGYAWVD | Carbonyl dic | CCl2O | Y | - | - | ClC(Cl)=O | 489 | Y | - | 9.994E-16 | 13.0711 |
| 18 | 2032-65-7 | CAS-RN | DTXSID30 | Methiocarb | 2032-65-7 | YFBPRJGD | 3,5-Dimethy | C11H15NO2 | Y | 18.14 | 88/485 | CNC(=O)OC | 65 | - | - | 1.446E-11 | 34.1692 |
| 19 | 2778-04-3 | CAS-RN | DTXSID20 | Endothion | 2778-04-3 | YCAGGFXS | S-[(5-Metho | C9H13O6PS | Y | - | - | COC1=COC | - | - | - | 4.355E-11 | 1.18341 |
| 20 | 12108-13-3 | CAS-RN | DTXSID90 | (Methylcyclc | 12108-13- | YASXMYPV | Tricarbonyl( | C9H7MnO3 | Y | 2.56 | 11/430 | - | 68 | - | - | - | - |
| 21 | 7803-51-2 | CAS-RN | DTXSID20 | Phosphine | 7803-51-2 | XYFCBTPG | Phosphane | H3P | Y | - | - | - | 928 | Y | - | - | - |
| 22 | 107-18-6 | CAS-RN | DTXSID80 | Allyl alcohol | 107-18-6 | XXROGKLT | Prop-2-en-1 | C3H6O | Y | 3.99 | 17/426 | OCC=C | 627 | Y | Y | 2.592E-11 | 4.03901 |
| 23 | 108-05-4 | CAS-RN | DTXSID30 | Vinyl acetate | 108-05-4 | XTXRWKR | Ethenyl acet | C4H6O2 | Y | 1.7 | 4/235 | CC(=O)OC= | 206 | Y | - | 2.5E-11 | 5.52157 |
| 24 | 19624-22-7 | CAS-RN | DTXSID10 | Pentaborane | 19624-22- | XPIBKKWN | - | B5H9 | Y | - | - | - | - | - | - | - | - |
| 25 | 75-74-1 | CAS-RN | DTXSID00 | Tetramethyl | 75-74-1 | XOOGZRUI | Tetramethyl | C4H12Pb | Y | - | - | C[Pb](C)(C) | 24 | - | - | - | - |

Worksheet1

# Send to batch and select….

**Intrinsic And Predicted Properties**

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

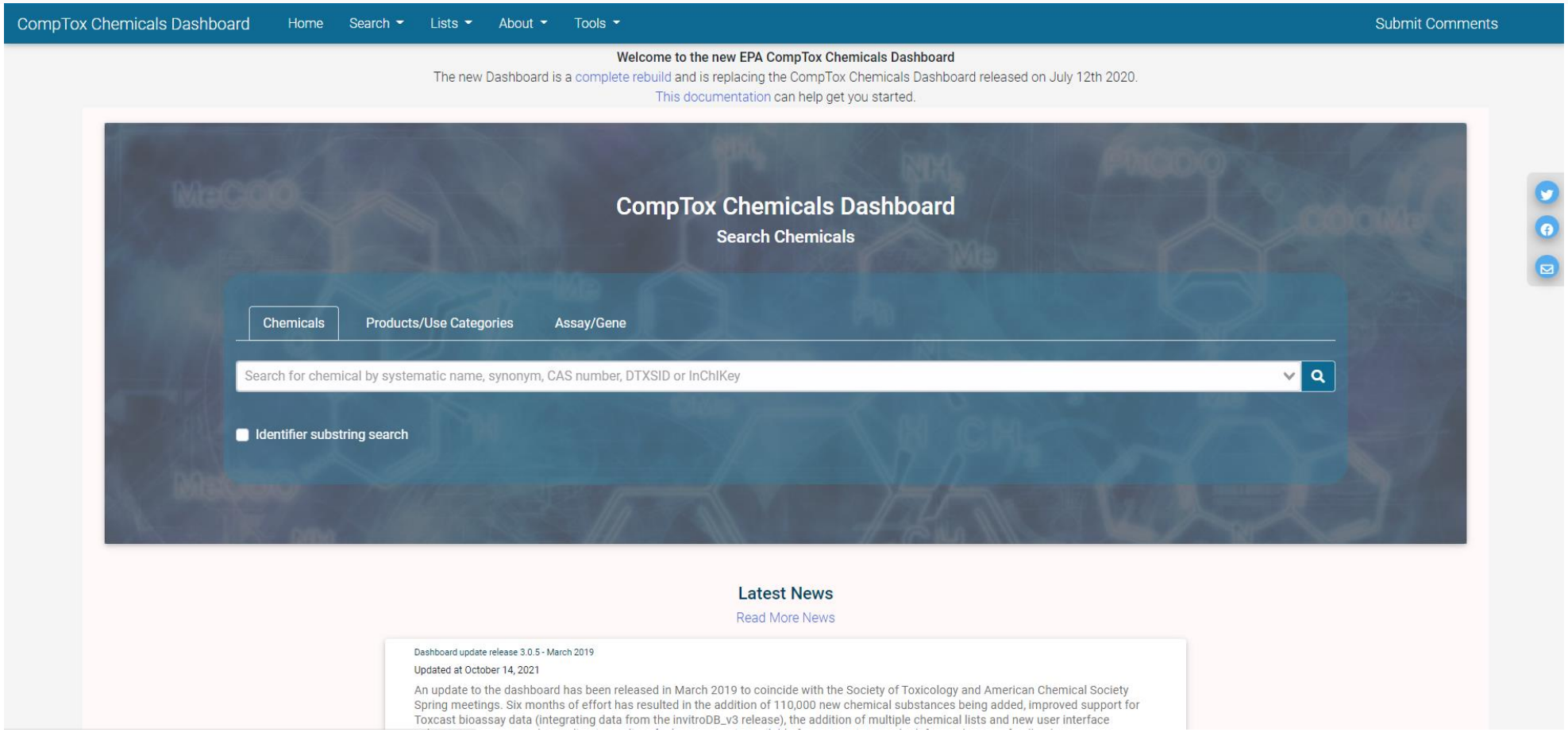
**Metadata**

- ☐ Curation Level Details
- ☐ NHANES/Predicted Exposure
- ☐ Data Sources
- ☐ Include ToxVal Data Availability
- ☐ Assay Hit Count
- ☐ Number of PubMed Articles
- ☐ PubChem Data Sources
- ☐ CPDat Product Occurrence Count
- ☐ IRIS
- ☐ PPRTV

- A few seconds to assemble
  - ToxCast data - #actives/#assays and % active
  - # articles in PubMed
  - Links to IRIS or PPRTV reports
  - TEST or OPERA predictions
  - Exposure data: predictions and CPDat

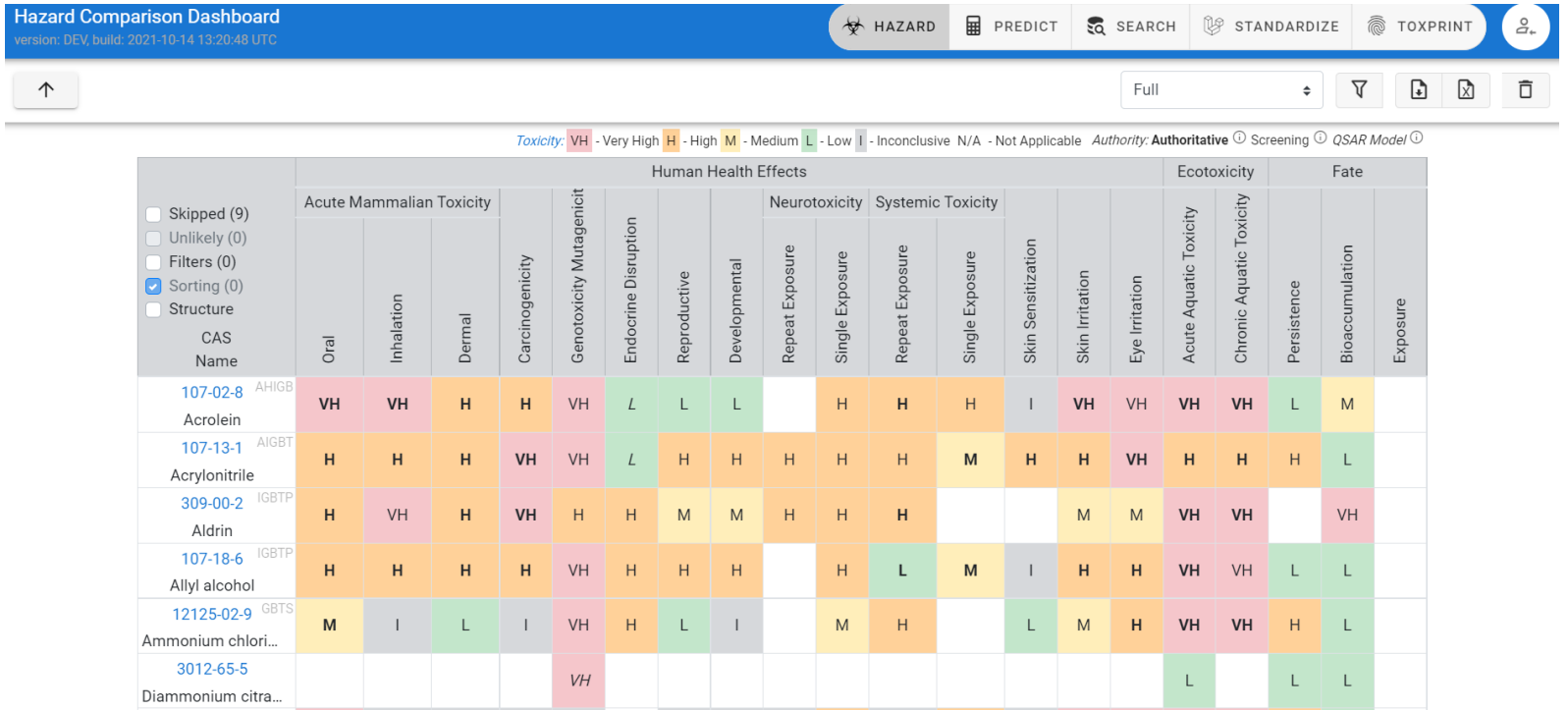
| DTXSID | PREFERRED_NAME | EXPOCAST_MEI | EXPOCAST | NHANES | TOXVAL_DATA | TOXCAST_%_ACT | TOXCAST_ | #PUBMED_ | PUBCHEM_ | CPDAT_COUI | IRIS_LINK | PPRTV_LINK |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| DTXSID2021105 | Pentachloronitrobenzene | 1.14e-07 | Y | Y | Y | 11.8 | 99/839 | 69 | 96 | 164 | Y | - |
| DTXSID4022527 | Propylparaben | 1.4e-05 | Y | Y | Y | 13.77 | 99/719 | 201 | 121 | 1476 | - | - |
| DTXSID4024064 | Dinex | 8.29e-08 | Y | - | Y | 42.13 | 99/235 | - | 35 | 5 | Y | - |
| DTXSID0032493 | Triadimenol | 1.73e-08 | Y | - | Y | 10.54 | 98/930 | 163 | 74 | 83 | - | - |
| DTXSID4032667 | Esfenvalerate | 1.7e-06 | Y | - | Y | 11.45 | 98/856 | 483 | 45 | 198 | - | - |
| DTXSID6020561 | Endrin | 1.29e-07 | Y | - | Y | 14.02 | 98/699 | 284 | 16 | 98 | Y | Y |
| DTXSID6025355 | Glutaraldehyde | 2.03e-05 | Y | - | Y | 14.35 | 98/683 | 6515 | 139 | 1144 | - | - |
| DTXSID8032417 | Isofenphos | 1.87e-08 | Y | - | Y | 16.28 | 98/602 | 30 | 42 | 60 | - | - |
| DTXSID6032352 | Chlorpyrifos-methyl | 1.07e-07 | Y | Y | Y | 11.27 | 97/861 | 72 | 50 | 116 | - | - |
| DTXSID8020620 | Fenthion | 8.99e-08 | Y | Y | Y | 11.56 | 97/839 | 354 | 100 | 99 | - | - |
| DTXSID2020189 | FD&C Blue No. 1 | 0.000178 | Y | - | Y | 13.72 | 97/707 | 174 | 49 | 672 | - | - |
| DTXSID7044843 | Erythrosin B | 6.3e-07 | Y | - | - | 24.25 | 97/400 | 14843 | 51 | 7 | - | - |
| DTXSID5041778 | Chloropropylate | 1.05e-07 | Y | - | Y | 40.93 | 97/237 | - | 36 | 12 | - | - |
| DTXSID5023900 | Benomyl | 1.11e-07 | Y | - | Y | 11.23 | 96/855 | 476 | 91 | 105 | Y | - |
| DTXSID9020247 | Carbaryl | 5.61e-08 | Y | Y | Y | 11.51 | 96/834 | 1135 | 117 | 245 | Y | - |
| DTXSID8024109 | Flutolanil | 1.63e-08 | Y | - | Y | 11.4 | 95/833 | 6 | 59 | 80 | - | - |
| DTXSID1023998 | Cypermethrin | 1.62e-06 | Y | Y | Y | 10.78 | 94/872 | 1148 | 148 | 246 | - | - |
| DTXSID2024242 | Paclobutrazol | 9.19e-08 | Y | - | Y | 11.11 | 94/846 | 139 | - | 40 | Y | - |
| DTXSID1020807 | 2-Mercaptobenzothiazole | 4.7e-05 | Y | - | Y | 12.82 | 94/733 | 111 | 181 | 86 | - | Y |

# Coming Soon….NEW DASHBOARD https://ccte-ccd.epa.gov/dashboard/

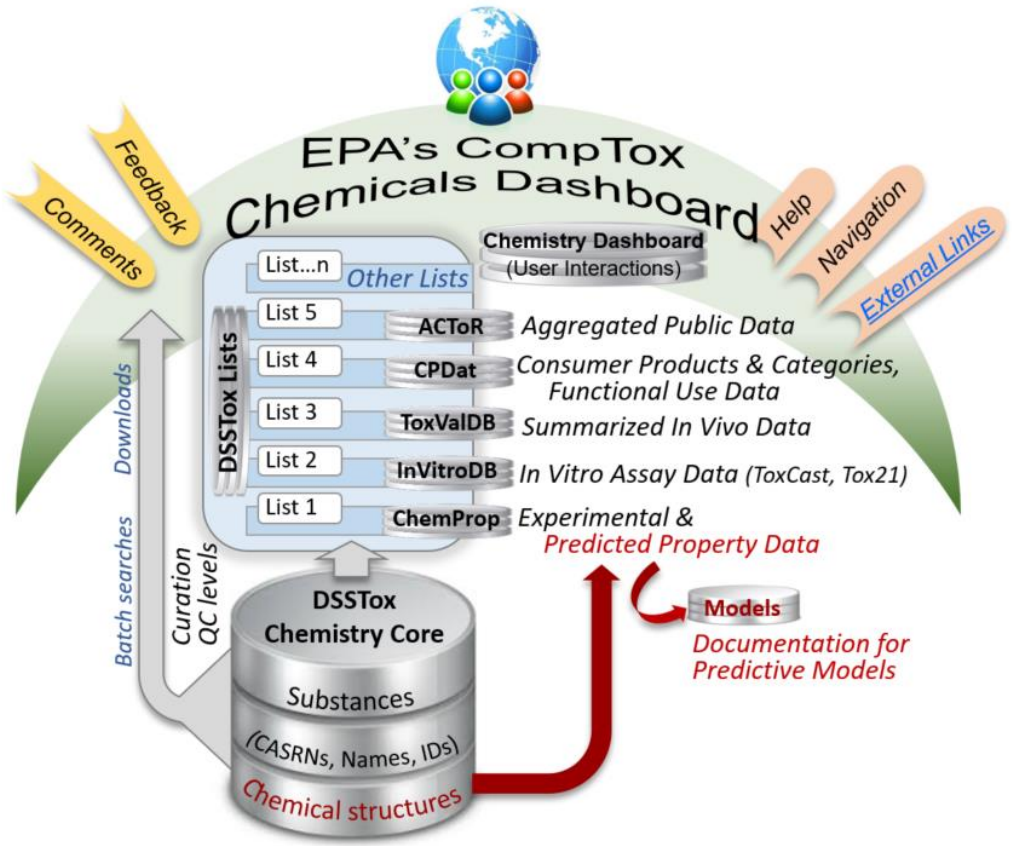


# Proof-of-Concept Apps

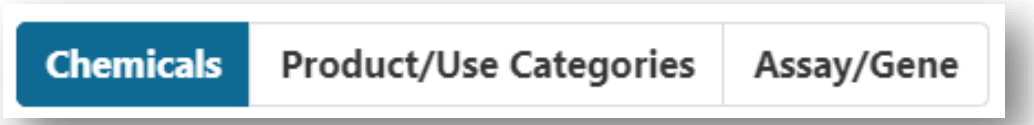
- Structure-substructure-similarity searching of Dashboard
- Batch prediction of physicochemical properties and toxicity
- “Hazard Comparison Dashboard” for comparing hazard profiles for chemicals



# Summary and Conclusion

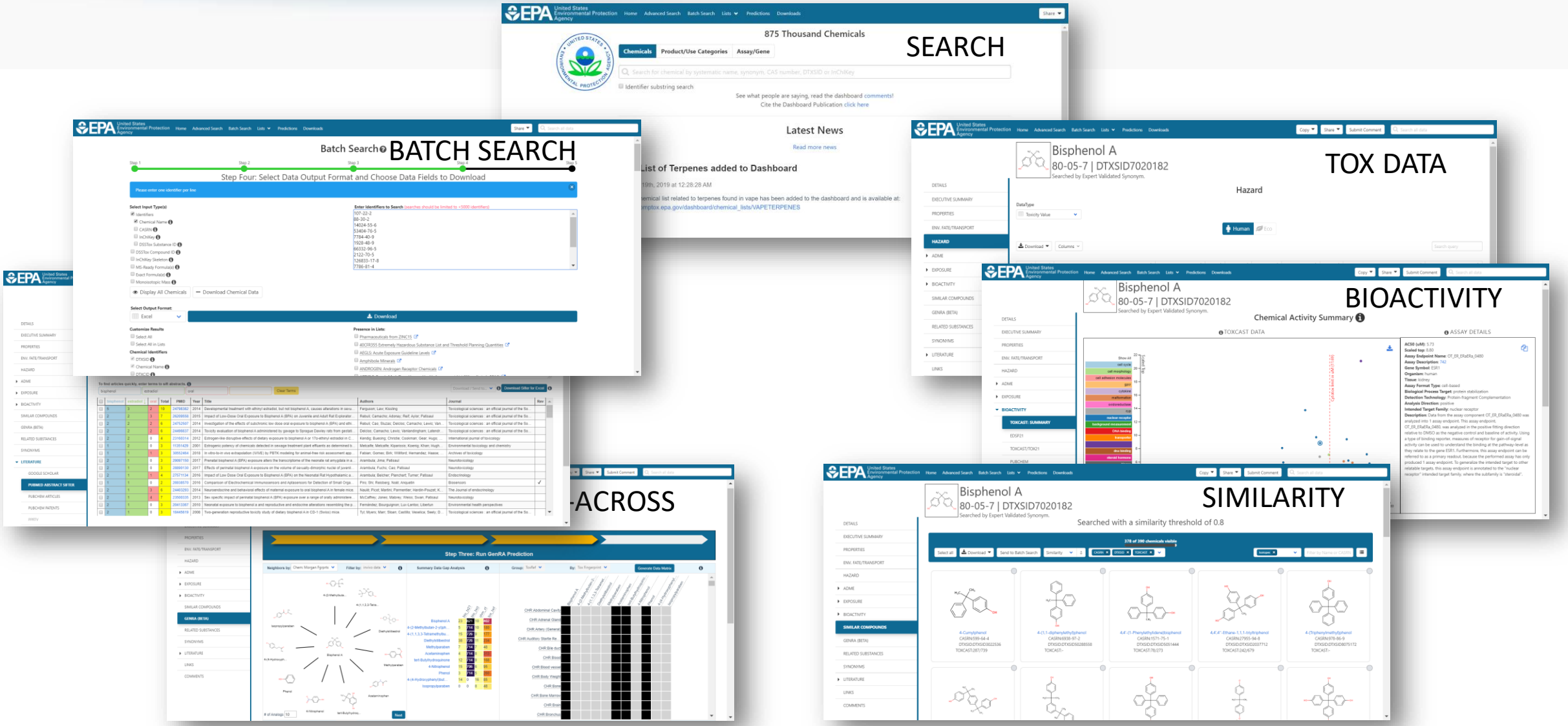



- CompTox Chemicals Dashboard - a central hub for environmental data
  - ~875k chemical substances
  - Integrating property data, hazard data, exposure data, *in vitro* bioactivity data
  - Interrogation of bioactivity data -
  - Multiple types of searches



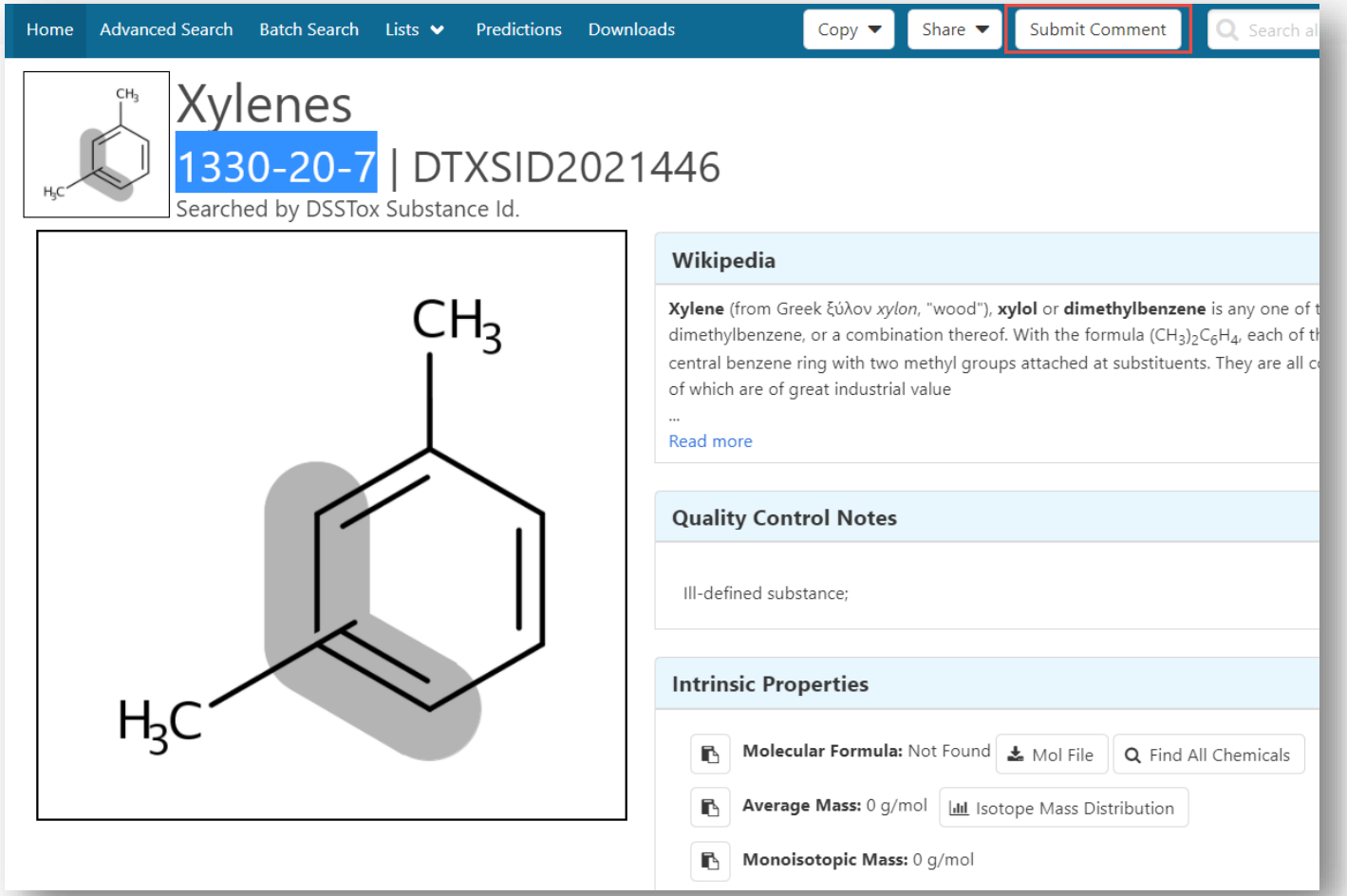

  - Batch search for thousands of chemicals
  - Real-time property and toxicity predictions
  - Downloadable files – CSV, TSV and Excel

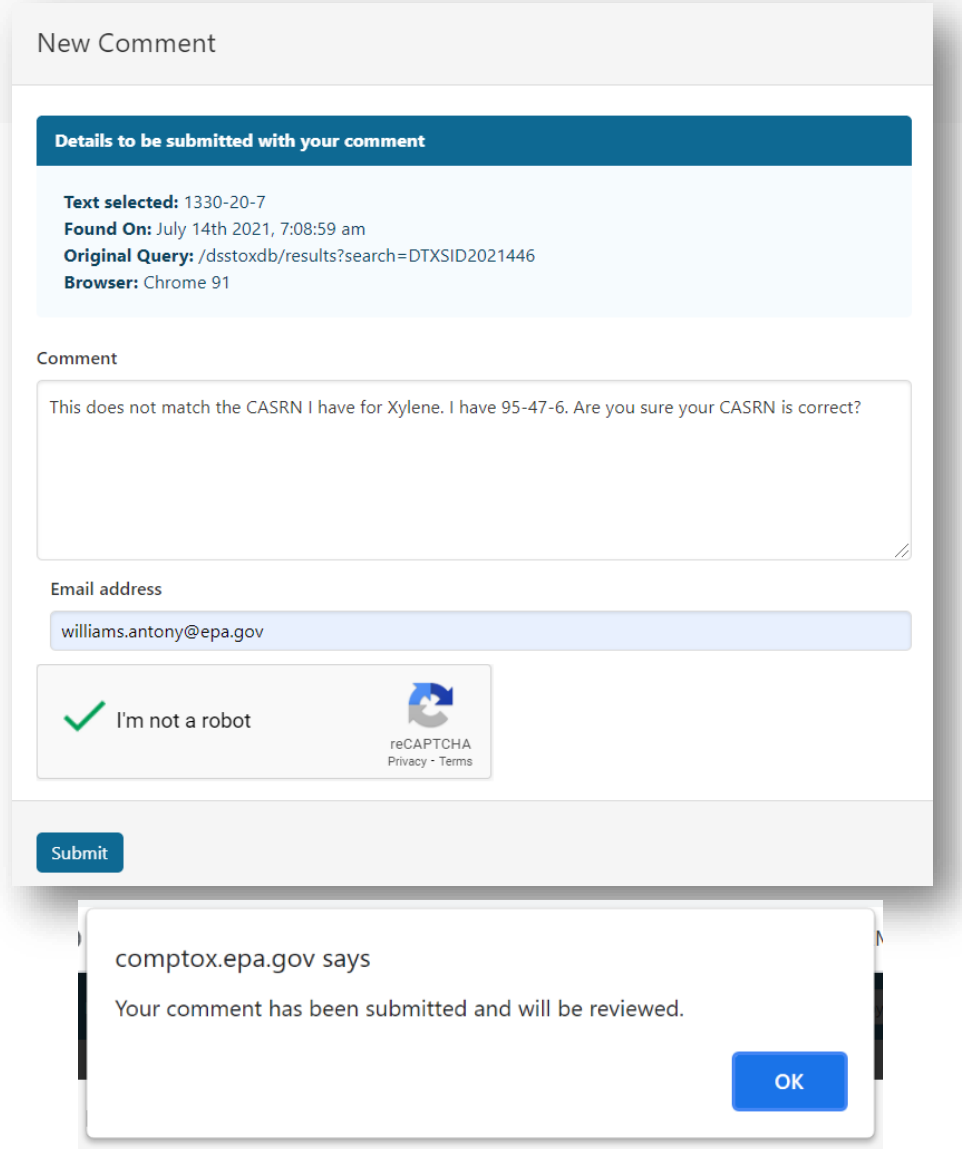
# CompTox Chemicals Dashboard
# https://comptox.epa.gov/dashboard



# If you find an error, or want to comment…
# Select text and “Submit Comment”

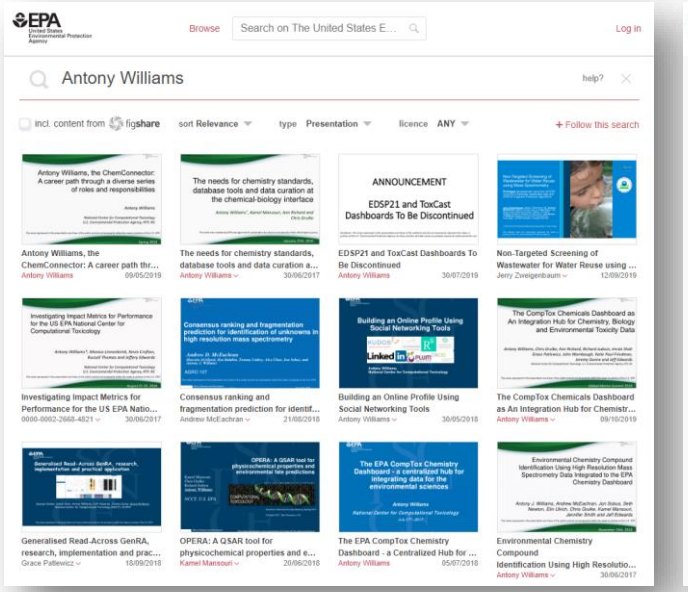
EPA United States Environmental Protection Agency

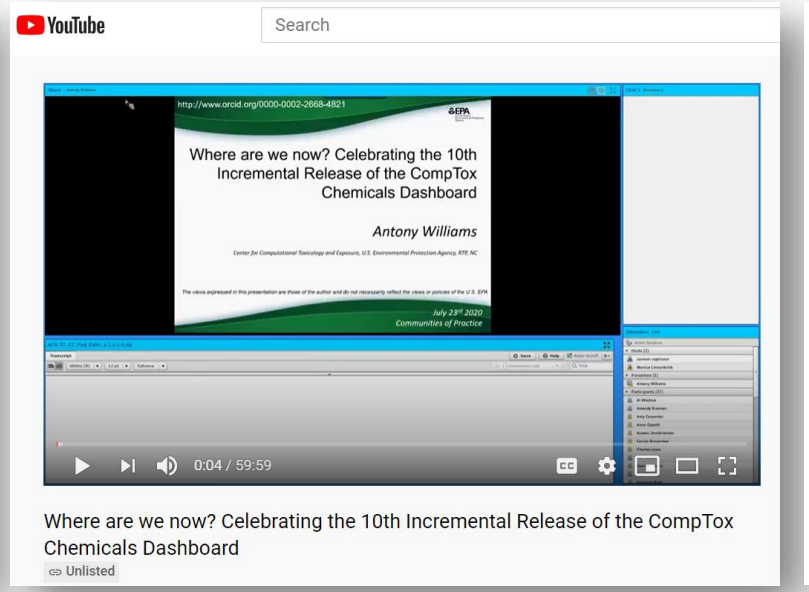


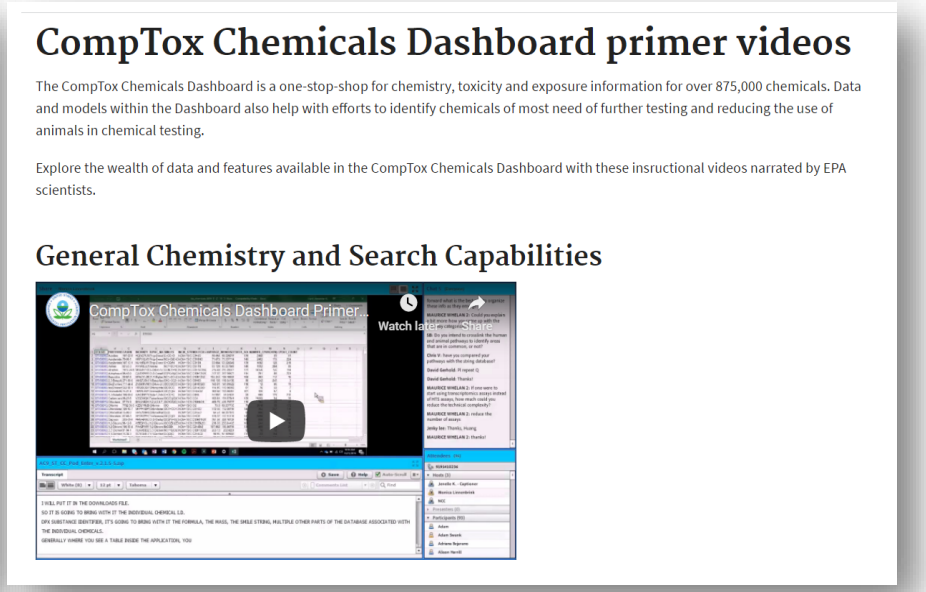



# You want to know more…

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



# Acknowledgments

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

EPA's Center for Computational Toxicology and Exposure