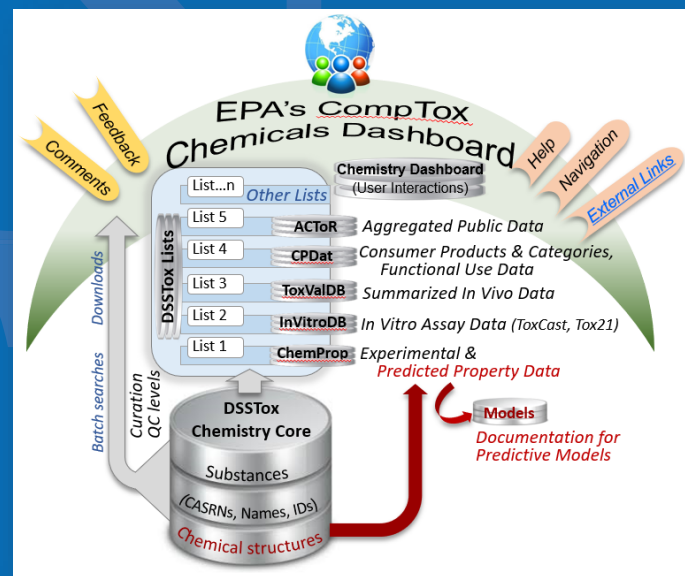


# UNC Chapel Hill Webinar: US-EPA Chemicals Dashboard – an integrated data hub for environmental science

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US EPA Office of Research and Development

September 2nd, 2020



# Approach

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

# EPA's CompTox Chemicals Dashboard

## A publicly accessible website delivering:

- ~882,000 chemicals with related property data
- Experimental and predicted physicochemical property data
- Integration to “biological assay data” for 1000’s of chemicals
- Information regarding consumer products containing chemicals
- Links to other agency websites and public data resources
- “Literature” searches for chemicals using public resources
- “Batch searching” for thousands of chemicals
- Downloadable Open Data for reuse and repurposing
- Many features (only highlighting a few)
- Access to multiple tools for multiple disciplines

# A single app integrating...

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875 Thousand Chemicals

**SEARCH**

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

Identifier substring search

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**BATCH SEARCH**

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

Please enter one identifier per line

Select Input Type(s):

- ☒ Identifiers
- ☐ Chemical Name(s)
- ☐ CASRN
- ☐ InChIKey
- ☐ DTXSID Substance
- ☐ DDTSC Compound
- ☐ InChIkey Substance
- ☐ MS-Ready Formula(s)
- ☐ Exact Formula(s)
- ☐ Monoisotopic Mass

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

107-26-2  
88-39-2  
14024-55-6  
33468-75-5  
7784-40-9  
1933-40-9  
60332-96-5  
2122-76-5  
126833-17-8  
7786-81-4

Download Chemical Data

Select Output Format:

- ☒ Excel
- ☐ CSV

Customize Results:

- ☒ Select All
- ☐ Select All in Lists

Chemical Identifiers:

- ☒ Chemical Name(s)
- ☐ DTXSID
- ☐ InChIKey

Presence in Lists:

- ☐ Pharmaceuticals from DTNCT
- ☐ ACRF655 Extremely Hazardous Substance List and Threshold Planning Quantities
- ☐ AEGU: Acute Exposure Guideline Levels
- ☐ Amphibols Minerals
- ☐ AROGEN: Androgen Receptor Chemistry

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**TOX DATA**

Bisphenol A  
80-05-7 | DTXSID7020182  
Searched by Expert Validated Synonym.

Hazard

Download Columns

Max	Type	Subtype	Risk assessment class	Value	Units	Study type	Exposure route	Species	Substance	Source
MES	Short-term	Critical Air	short-term	500	mg/m3	-	inhalation	-	TG 230 Military Exposure Guidelines Table	OOD
MES	Short-term	Marginal Air	short-term	100	mg/m3	-	inhalation	-	TG 230 Military Exposure Guidelines Table	OOD
MES	Short-term	Neighborhood Air	short-term	15	mg/m3	-	inhalation	-	TG 230 Military Exposure Guidelines Table	OOD
MES	Soil	Negligible Soil	chronic	100000	mg/kg	-	soil	-	TG 230 Military Exposure Guidelines Table	OOD
MES	Long-term	Soil Negligible Water	chronic	7	mg/L	-	oral	-	TG 230 Military Exposure Guidelines Table	OOD

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**BIOACTIVITY**

Chemical Activity Summary

Bisphenol A  
80-05-7 | DTXSID7020182  
Searched by Expert Validated Synonym.

TOXCAST DATA

ASSAY DETAILS

ACSR (pM): 5.73  
Scaled log: 8.31  
Assay Description: 742  
Gene Symbol: ESR1  
Organism: human  
Tissue: Uterine  
Assay Format: Type: cell-based  
Biological Process: Target: protein stabilization  
Detection Technology: Western Blotting  
Analysis Direction: positive  
Intended Target Family: nuclear receptor  
Description: Data from this assay component OT\_ER\_ESR1a\_D480 was analyzed into 1 assay endpoint. OT\_ER\_ESR1a\_D480 was analyzed in the positive filtering direction relative to DMSO as the negative control and baseline of activity. Using a type of binding reporter, measure of receptor for gene of signal activity can be used to understand the binding at the pathway level as this relates to the gene ESR1. Furthermore, this assay endpoint can be referred to as a primary readout, because the performed assay has only produced 1 assay endpoints. To generalize the intended target to other suitable targets, this assay endpoint is associated to the "nuclear receptor" intended target family, where the subfamily is "steroidal".

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**SIMILARITY**

Bisphenol A  
80-05-7 | DTXSID7020182  
Searched by Expert Validated Synonym.

Searched with a similarity threshold of 0.8

376 of 399 chemicals visible

Download Send to Batch Search Similarity

4-Cumylphenol  
CASRN:81-77-1  
DTXSID:DTXSID0022556  
TOXCAT:706779

4-(1,1-diphenylethyl)phenol  
CASRN:81-77-1  
DTXSID:DTXSID008858  
TOXCAT:706779

4,4'-[1,1-bis(4-phenyl)ethane]diphenol  
CASRN:2795-41-8  
DTXSID:DTXSID00712  
TOXCAT:4240679

4,4'-[1,1-bis(4-phenyl)ethane]diphenol  
CASRN:2795-41-8  
DTXSID:DTXSID00712  
TOXCAT:4240679

4-chlorophenylphenol  
CASRN:81-77-1  
DTXSID:DTXSID00712  
TOXCAT:4240679

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Antony Williams  
National Center for Computational Toxicology  
U.S. Environmental Protection Agency, 4705 MC  
Spring 2018

Antony Williams, the ChemConnector: A career path thr...  
Antony Williams 09/05/2019

**The needs for chemistry standards, database tools and data curation at the chemical-biology interface**  
Antony Williams\*, Kamel Mansouri, Ann Richard and Chris Grulke  
January 2016

The needs for chemistry standards, database tools and data curation a...  
Antony Williams 30/06/2017

**ANNOUNCEMENT**  
**EDSP21 and ToxCast Dashboards To Be Discontinued**  
January 2016

EDSP21 and ToxCast Dashboards To Be Discontinued  
Antony Williams 30/07/2019

**Non-Targeted Screening of Wastewater for Water Reuse using Mass Spectrometry**  
Jerry Zweigenbaum  
12/09/2019

**Investigating Impact Metrics for Performance for the US EPA National Center for Computational Toxicology**  
Antony Williams\*, Monica Linsenbrink, Kevin Crofton, Russell Thomas and Jeffery Edwards  
National Center for Computational Toxicology  
U.S. Environmental Protection Agency, 4705 MC  
August 22-26, 2018

Investigating Impact Metrics for Performance for the US EPA Natio...  
0000-0002-2668-4821 30/06/2017

**Consensus ranking and fragmentation prediction for identification of unknowns in high resolution mass spectrometry**  
Andrew D. McEachran  
Hassam McLeod, Osa Bullock, Finlay Cullen, Alex Chan, Jon Sobus, and Anthony J. Williams  
AGRO 197  
November 2018

Consensus ranking and fragmentation prediction for identif...  
Andrew McEachran 21/08/2018

**Building an Online Profile Using Social Networking Tools**  
Antony Williams  
National Center for Computational Toxicology  
July 2017

Building an Online Profile Using Social Networking Tools  
Antony Williams 30/05/2018

**The CompTox Chemicals Dashboard as An Integration Hub for Chemistry, Biology and Environmental Toxicity Data**  
Antony Williams, Chris Grulke, Ann Richard, Richard Judson, Jerrisa Shih, Grace Pattlewicz, John Wambaugh, Katie Paul-Friedman, Jeremy Dunne and Jeff Edwards  
National Center for Computational Toxicology, U.S. Environmental Protection Agency, 4705 MC  
Global Meeting Summer 2018

The CompTox Chemicals Dashboard as An Integration Hub for Chemistr...  
Antony Williams 09/10/2019

**Generalised Read-Across GenRA, research, implementation and practical application**  
Grace Pattlewicz  
18/09/2018

**OPERA: A QSAR tool for physicochemical properties and environmental fate predictions**  
Kamel Mansouri  
Chris Grulke  
Richard Judson  
Michele M. Wilson  
NCCCT, U.S. EPA  
COMPUTATIONAL TOXICOLOGY  
November 2017

OPERA: A QSAR tool for physicochemical properties and e...  
Kamel Mansouri 20/06/2018

**The EPA CompTox Chemistry Dashboard - a centralized hub for integrating data for the environmental sciences**  
Antony Williams  
National Center for Computational Toxicology  
July 2017

The EPA CompTox Chemistry Dashboard - a Centralized Hub for ...  
Antony Williams 05/07/2018

**Environmental Chemistry Compound Identification Using High Resolution Mass Spectrometry Data Integrated to the EPA Chemistry Dashboard**  
Antony J. Williams, Andrew McEachran, Jon Sobus, Seth Newton, Erin Ulrich, Chris Grulke, Kamel Mansouri, Jennifer Smith and Jeff Edwards  
November 14th, 2018

Environmental Chemistry Compound Identification Using High Resolutio...  
Antony Williams 30/06/2017

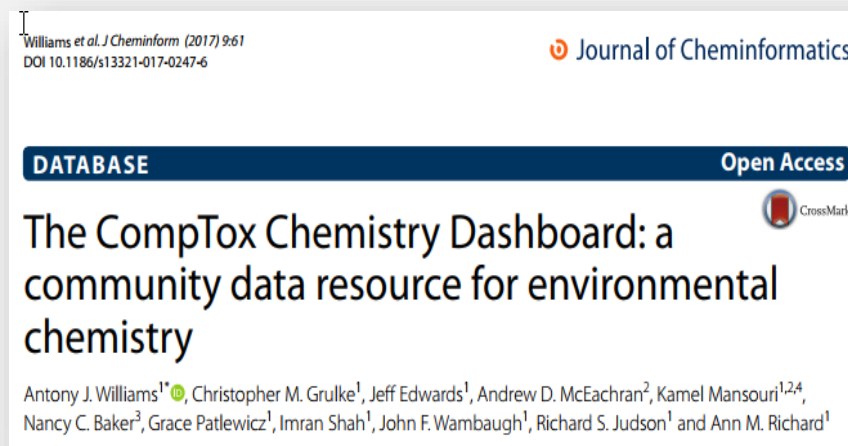
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