

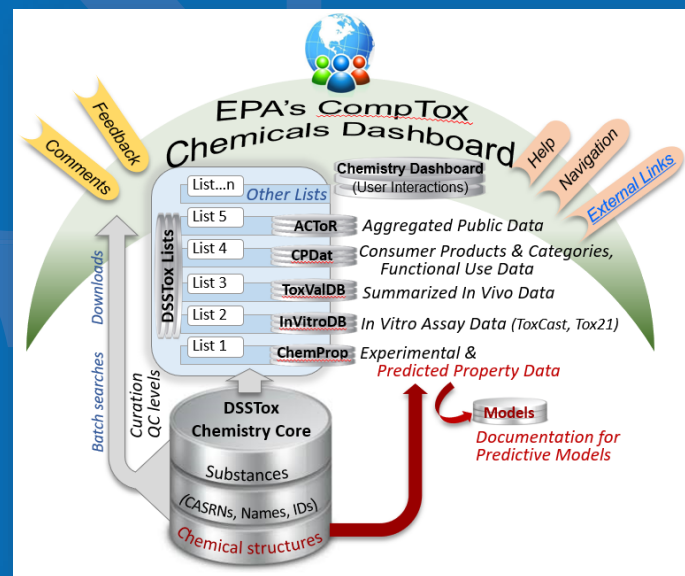
EPA Tools & Resources Training Webinar:

EPA's CompTox Chemicals Dashboard – *Data Integration Hub for Environmental Chemistry Data*

Antony Williams

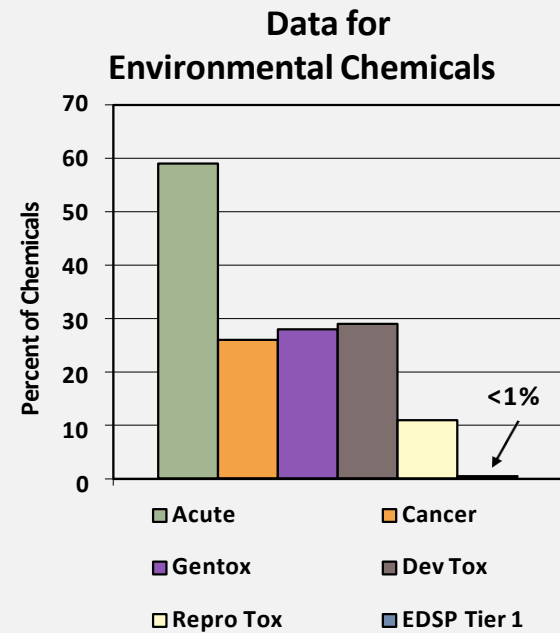
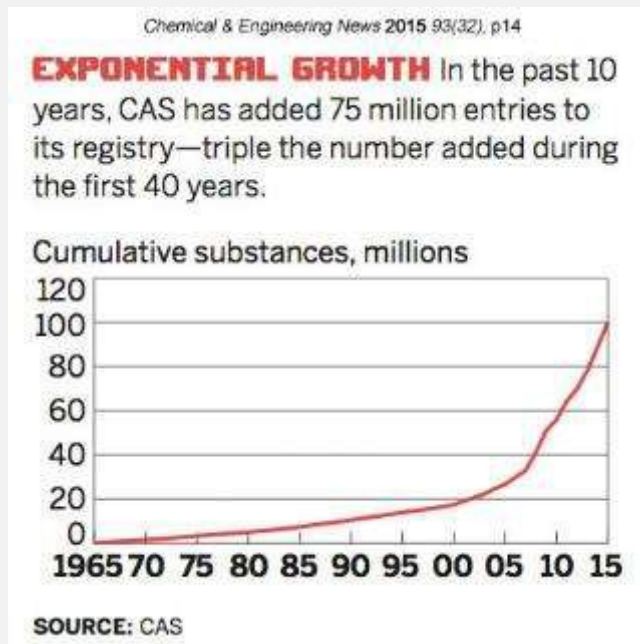
Center for Computational Toxicology and Exposure
US EPA Office of Research and Development

June 3, 2020



Problem: Too Many Chemicals, Too Few Resources

- Timely characterization of human and ecological risk posed by thousands of existing and emerging chemicals is a critical challenge to protect public health and the environment



Modified from Judson *et al.*, EHP 2010

*CAS – Chemical Abstracts Service

Approach

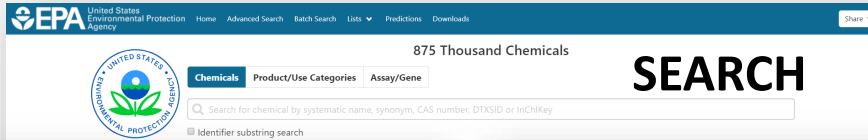
- **Develop a “first-stop-shop” for data as an integration node for environmental chemical data to support EPA and partner decision-making:**
 - Centralized location for relevant chemical data
 - Chemistry, exposure, hazard, dosimetry
 - Combination of existing data and predictive models
 - Publicly 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:

- ~875,000 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 (direct data interpolation and predictive) for multiple disciplines

A single app integrating...



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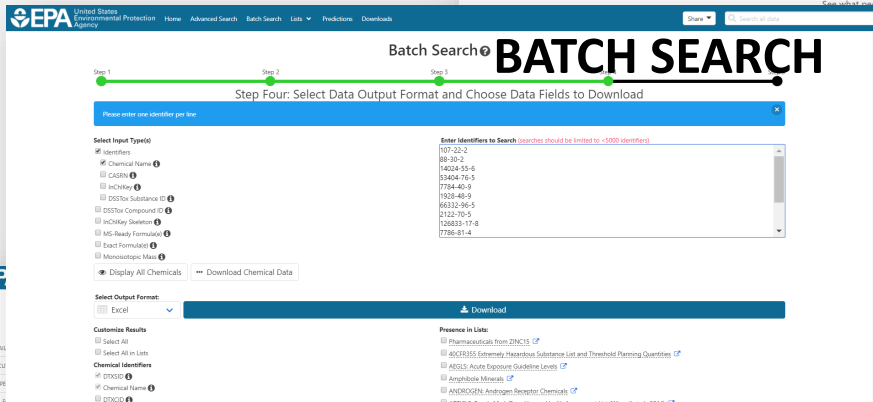
875 Thousand Chemicals

Chemicals Product/Use Categories Assay/Gene

SEARCH

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

Identifier substring search



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Batch Search **BATCH SEARCH**

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

Enter one or more identifier per line

Select Input Type(s)

- Identifiers
 - 107-26-2
 - 88-39-2
 - 14208-55-6
 - 33464-76-5
 - 7784-40-9
 - 1928-40-9
 - 6632-96-5
 - 2129-70-5
 - 12683-17-8
 - 7786-81-4

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

Select Output Format

Download

Customize Results

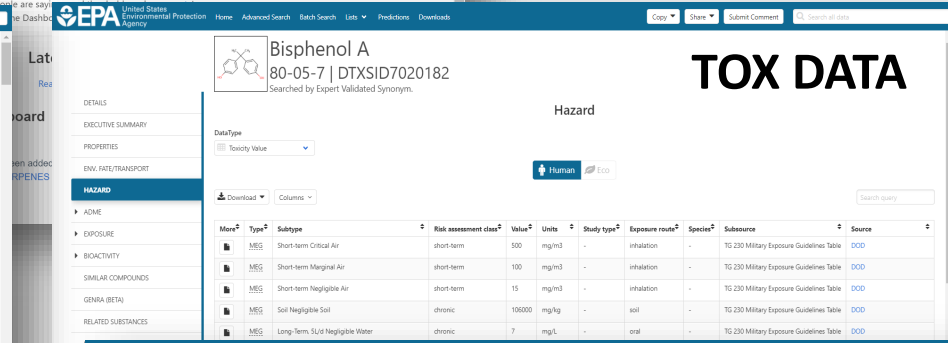
- Select All
- Select All in Lists

Chemical Identifiers

- DTXSID
- Chemical Name
- SYNOPSIS

Previews in Lists:

- Pharmaceutical from DTXSID
- ACQF655 Extremely Hazardous Substance List and Threshold Planning Quantities
- ARSD: Acute Exposure Guideline Levels
- Amphibols Minerals
- ANERGEM Androgen Receptor Chemicals



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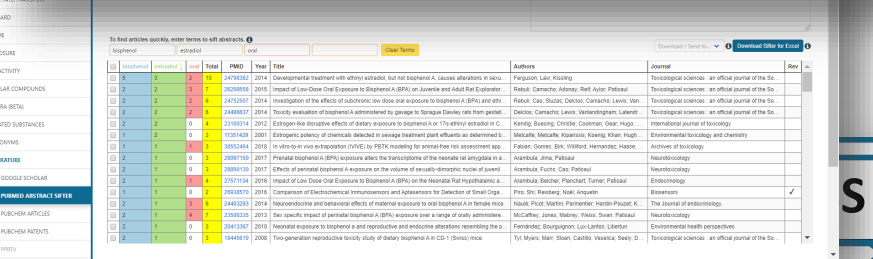
Bisphenol A
80-05-7 | DTXSID7020182
Searched by Expert Validated Synonym.

TOX DATA

Hazard

Download Columns

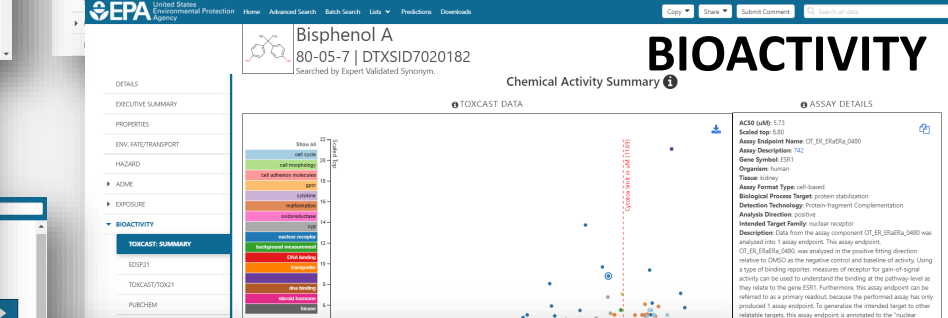
Max	Type	Subtype	Risk assessment class	Value	Units	Study type	Exposure route	Species	Substance	Source
MES	Short-term	Critical Air	short-term	500	mg/m3	-	inhalation	-	TQ 230 Military Exposure Guidelines Table	DOO
MES	Short-term	Marginal Air	short-term	100	mg/m3	-	inhalation	-	TQ 230 Military Exposure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



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To find articles quickly, enter terms to left abstracts

Document	Abstract	Title	Year	Author	Journal	View
2	1	2019	2019	Ferguson, Lee; Kissing	Toxicological sciences: an official journal of the So.	
2	2	2019	2019	Rehal, Carmelo; Adenry, Bett; Aizer, Paloma	Toxicological sciences: an official journal of the So.	
2	2	2014	2014	Rehal, Car, Szilag, Dorcas, Corvaci, Levis, San	Toxicological sciences: an official journal of the So.	
2	2	2014	2014	Decker, Catherine; Lewis, Vandenbroucke, Laurent	International journal of toxicology	
2	2	2012	2012	Kendig, Benjamin; Christie, Colleen; Oak, Hugo	Environmental toxicology and chemistry	
2	1	2010	2010	Makela, Marika; Kogut, Keating; Stein, Hugh	Archives of toxicology	
2	1	2009	2009	Avramovic, Goran; Birk, Wilfried; Hammer, Heide	Neurotoxicology	
2	1	2007	2007	Avramovic, Ana; Paltauf	Neurotoxicology	
2	1	2007	2007	Avramovic, Facha, Cas, Paltauf	Neurotoxicology	
2	1	2006	2006	Avramovic, Beatrice; Paltauf, Turner, Paltauf	Endocrinology	
2	1	2006	2006	Przybyl, Dorota; Paltauf, Turner, Paltauf	Endocrinology	
2	1	2004	2004	Nauk, Piotr; Martin, Pamphiler; Hardin-Pozdek, K.	The Journal of endocrinology	
2	1	2003	2003	McCarthy, James; Melny, Wynn; Stein, Paltauf	Neurotoxicology	
2	1	2003	2003	Franziska, Stepputat; Lutz, Lutz; Lutz	Environmental health perspectives	
2	1	2008	2008	Tu, Min; Mao, Shun; Cao, Wei; Yao, Sany; D.	Toxicological sciences: an official journal of the So.	



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

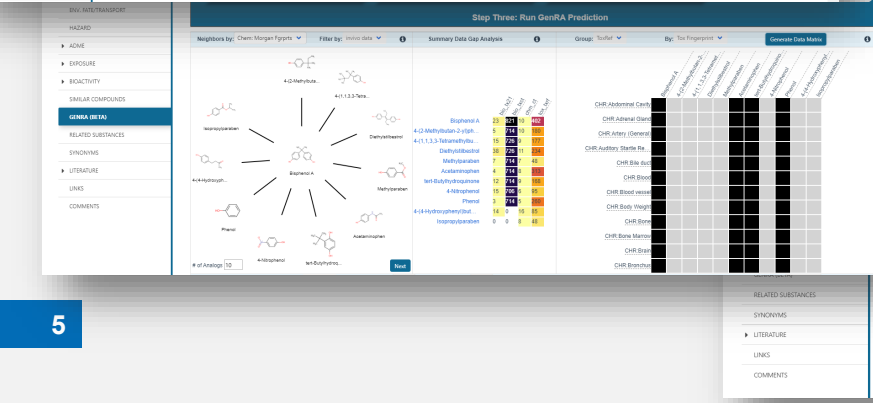
BIOACTIVITY

Chemical Activity Summary

TOXCAST DATA

ASSAY DETAILS

AC50 (µM): 5.73
Scaled Top: 5.00
Assay Endpoint Name: CT_ER_ESRRA_D4D
Assay Description: T42
Gene Symbol: ESR1
Organism: Human
Tissue: Spleen
Assay Format Type: Cell-based
Biological Process Target: protein stabilization
Detection Technology: Western Blotting/Complementation
Analysis Direction: positive
Intended Target Family: nuclear receptor
Description: Data from the assay component CT_ER_ESRRA_D4D was analyzed into 1 assay endpoint. This assay endpoint, CT_ER_ESRRA_D4D, was analyzed in the positive fitting direction relative to DMSO as the negative control and baseline of activity. Using a type of binding requires measure of receptor for gain-of-activity can be used to understand the binding of the path-way 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 endpoint. To generalize the intended target to other suitable targets, this assay endpoint is annotated to the "nuclear receptor" intended target family, where the suitability is "medium".



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

SIMILARITY

Searched with a similarity threshold of 0.8

378 of 399 chemicals visible

Download Send to Batch Search Similarity Color Sort Group Filter

Neighbors by: Chem Morgan Fingers Filter by: Index Data

Summary Data Gap Analysis

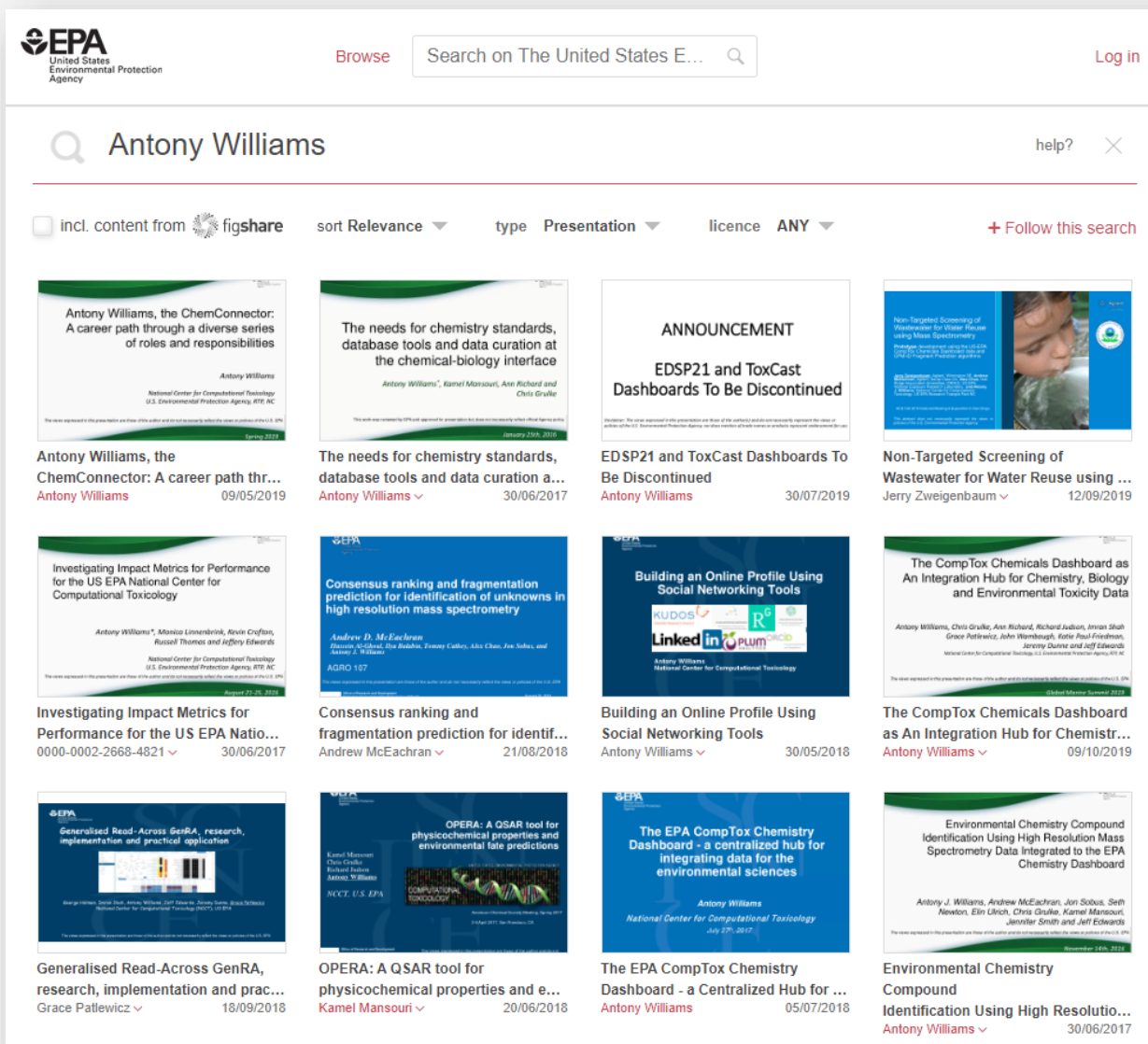
Chemical	DTXSID	Similarity	Group	Fingers
Bisphenol A	80-05-7	1.00	Group 1	100
4-(1,1,1-trifluoroethyl)phenol	CA98N751-1	0.98	Group 1	100
4-(1-phenyl-1,1,1-trifluoroethyl)phenol	CA98N751-4	0.98	Group 1	100
4,4'-[Thiara-1,1,1-trifluoroethyl]bisphenol	CA98N751-11	0.98	Group 1	100
4,4'-[Thiara-1,1,1-trifluoroethyl]bisphenol	CA98N751-12	0.98	Group 1	100
4,4'-[Thiara-1,1,1-trifluoroethyl]bisphenol	CA98N751-13	0.98	Group 1	100
4,4'-[Thiara-1,1,1-trifluoroethyl]bisphenol	CA98N751-14	0.98	Group 1	100
4,4'-[Thiara-1,1,1-trifluoroethyl]bisphenol	CA98N751-15	0.98	Group 1	100
4,4'-[Thiara-1,1,1-trifluoroethyl]bisphenol	CA98N751-16	0.98	Group 1	100
4,4'-[Thiara-1,1,1-trifluoroethyl]bisphenol	CA98N751-17	0.98	Group 1	100
4,4'-[Thiara-1,1,1-trifluoroethyl]bisphenol	CA98N751-18	0.98	Group 1	100
4,4'-[Thiara-1,1,1-trifluoroethyl]bisphenol	CA98N751-19	0.98	Group 1	100
4,4'-[Thiara-1,1,1-trifluoroethyl]bisphenol	CA98N751-20	0.98	Group 1	100

RELATED SUBSTANCES

- SYNOPSIS
- LITERATURE
- LINKS
- COMMENTS

Many Presentations Online

<https://tinyurl.com/w5hqs55>



The screenshot shows the EPA's presentation search interface. At the top left is the EPA logo. A search bar contains the text "Antony Williams". To the right of the search bar are "Browse" and "Log in" links. Below the search bar, there are filters for "incl. content from figshare", "sort Relevance", "type Presentation", and "licence ANY". A "Follow this search" button is also present. The main area displays a grid of 12 presentation thumbnails, each with a title, author list, and date. The presentations cover topics such as career paths, chemistry standards, dashboard discontinuation, wastewater screening, impact metrics, consensus ranking, social networking tools, and various chemical dashboards.

Title	Author(s)	Date
Antony Williams, the ChemConnector: A career path through a diverse series of roles and responsibilities	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 Grulle	30/06/2017
ANNOUNCEMENT 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	Andrew McEachran	30/06/2017
Consensus ranking and fragmentation prediction for identification of unknowns in high resolution mass spectrometry	Andrew McEachran	21/08/2018
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	09/10/2019
Generalised Read-Across GenRA, research, implementation and practical application	Grace Patelewicz	18/09/2018
OPERA: A QSAR tool for physicochemical properties and environmental fate predictions	Kamel Mansouri	20/06/2018
The EPA CompTox Chemistry Dashboard - a centralized hub for integrating data for the environmental sciences	Antony Williams	05/07/2018
Environmental Chemistry Compound Identification Using High Resolution Mass Spectrometry Data Integrated to the EPA Chemistry Dashboard	Antony Williams	30/06/2017

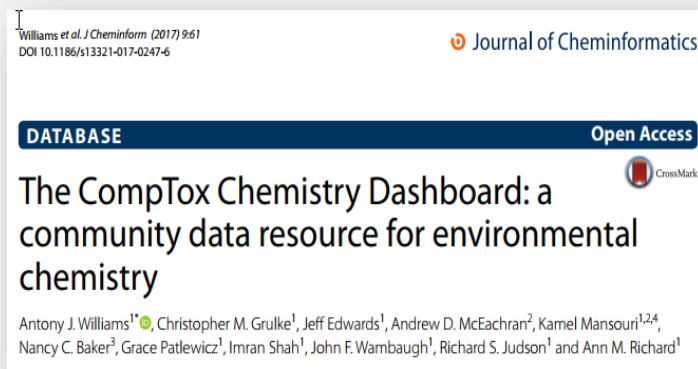
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US EPA Office of Research and Development

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

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