

# The US EPA CompTox Chemicals Dashboard website for Environmental Science Data

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*The views expressed in this presentation are those of the authors and do not necessarily reflect the views or policies of the U.S. EPA*

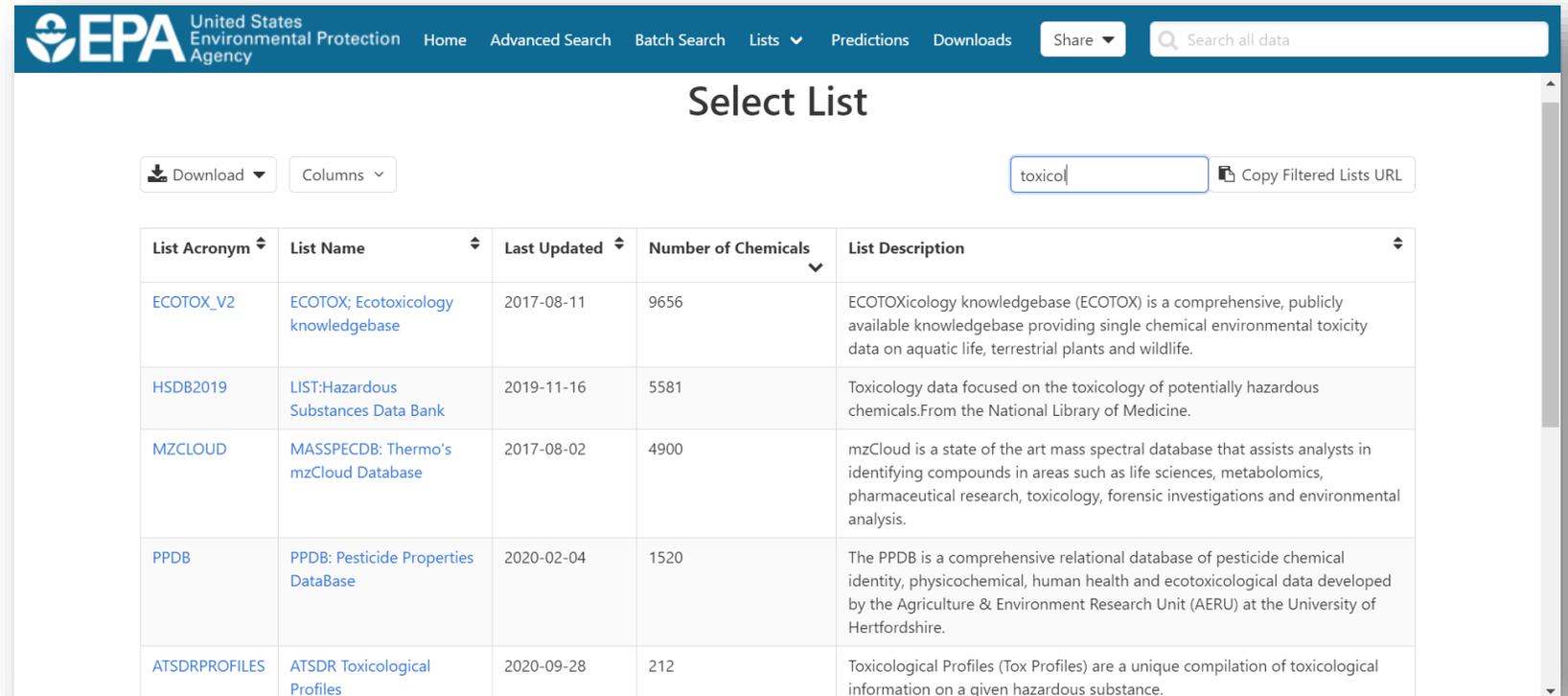
# Problem: Too Many Chemicals and Too Few Quality Data Resources

- **Fast characterization** of human and ecological **risk** posed by existing and emerging chemicals is a critical challenge
- **Easy access to data** improves efficiency and ultimately accelerates chemical risk assessment
- Develop a “**first-stop-shop**” for environmental chemical data to support US-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



# Focused Lists based on agency programs

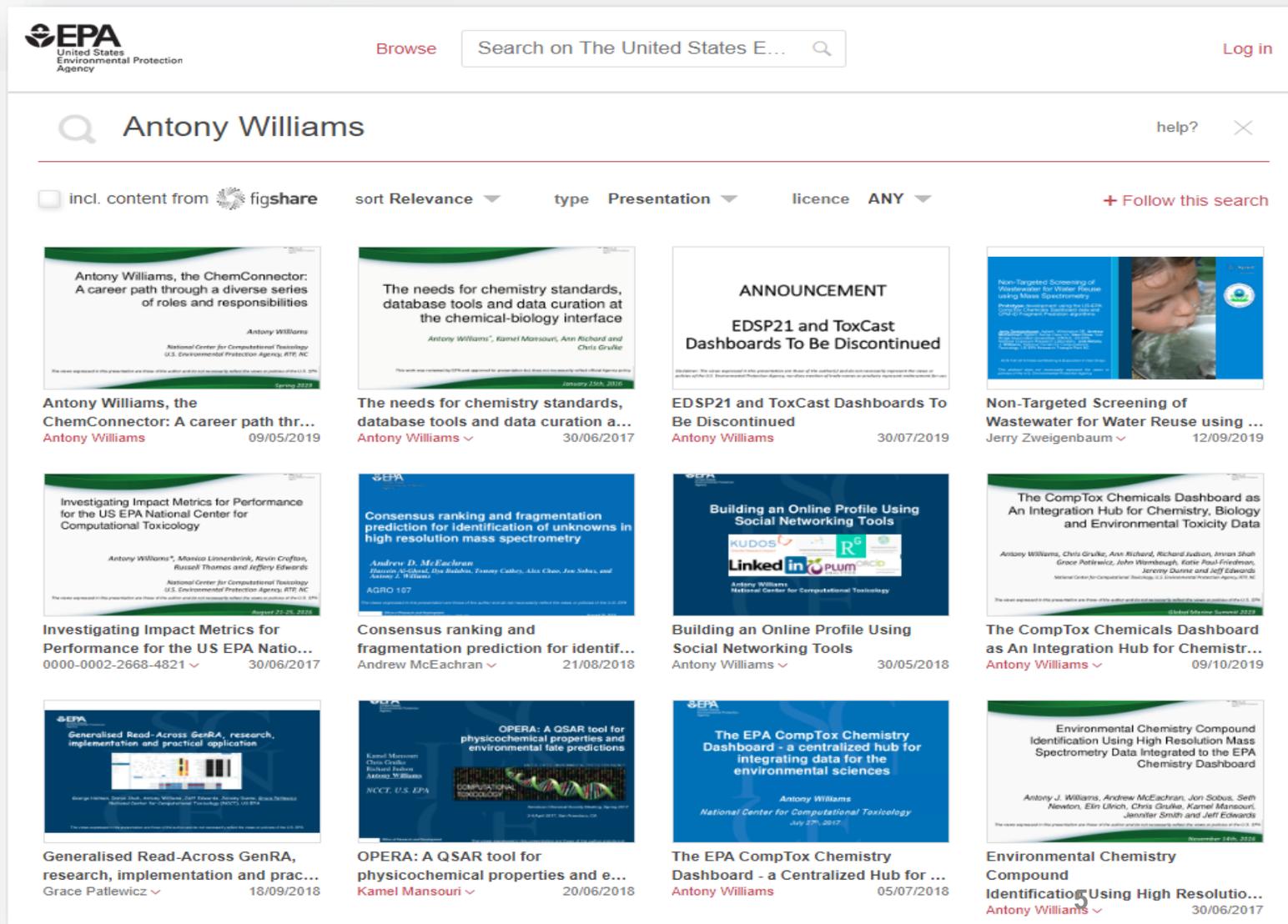
- Specific lists and collections of interest to the agency
  - Hydraulic fracturing
  - Disinfectant by-products
  - PFAS chemicals
  - TSCA inventory
  - Pesticides
  - etc...



The screenshot shows the EPA 'Select List' interface. At the top, there is a navigation bar with the EPA logo, 'United States Environmental Protection Agency', and links for Home, Advanced Search, Batch Search, Lists, Predictions, and Downloads. A search bar on the right contains the text 'toxico'. Below the navigation bar, the page title is 'Select List'. There are two dropdown menus: 'Download' and 'Columns'. A search input field contains 'toxico' and a 'Copy Filtered Lists URL' button is to its right. The main content is a table with the following columns: List Acronym, List Name, Last Updated, Number of Chemicals, and List Description.

List Acronym	List Name	Last Updated	Number of Chemicals	List Description
ECOTOX_V2	<a href="#">ECOTOX; Ecotoxicology knowledgebase</a>	2017-08-11	9656	ECOTOXicology knowledgebase (ECOTOX) is a comprehensive, publicly available knowledgebase providing single chemical environmental toxicity data on aquatic life, terrestrial plants and wildlife.
HSDB2019	<a href="#">LIST:Hazardous Substances Data Bank</a>	2019-11-16	5581	Toxicology data focused on the toxicology of potentially hazardous chemicals.From the National Library of Medicine.
MZCLOUD	<a href="#">MASSPECDB: Thermo's mzCloud Database</a>	2017-08-02	4900	mzCloud is a state of the art mass spectral database that assists analysts in identifying compounds in areas such as life sciences, metabolomics, pharmaceutical research, toxicology, forensic investigations and environmental analysis.
PPDB	<a href="#">PPDB: Pesticide Properties DataBase</a>	2020-02-04	1520	The PPDB is a comprehensive relational database of pesticide chemical identity, physicochemical, human health and ecotoxicological data developed by the Agriculture & Environment Research Unit (AERU) at the University of Hertfordshire.
ATSDRPROFILES	<a href="#">ATSDR Toxicological Profiles</a>	2020-09-28	212	Toxicological Profiles (Tox Profiles) are a unique compilation of toxicological information on a given hazardous substance.

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**EPA** United States Environmental Protection Agency

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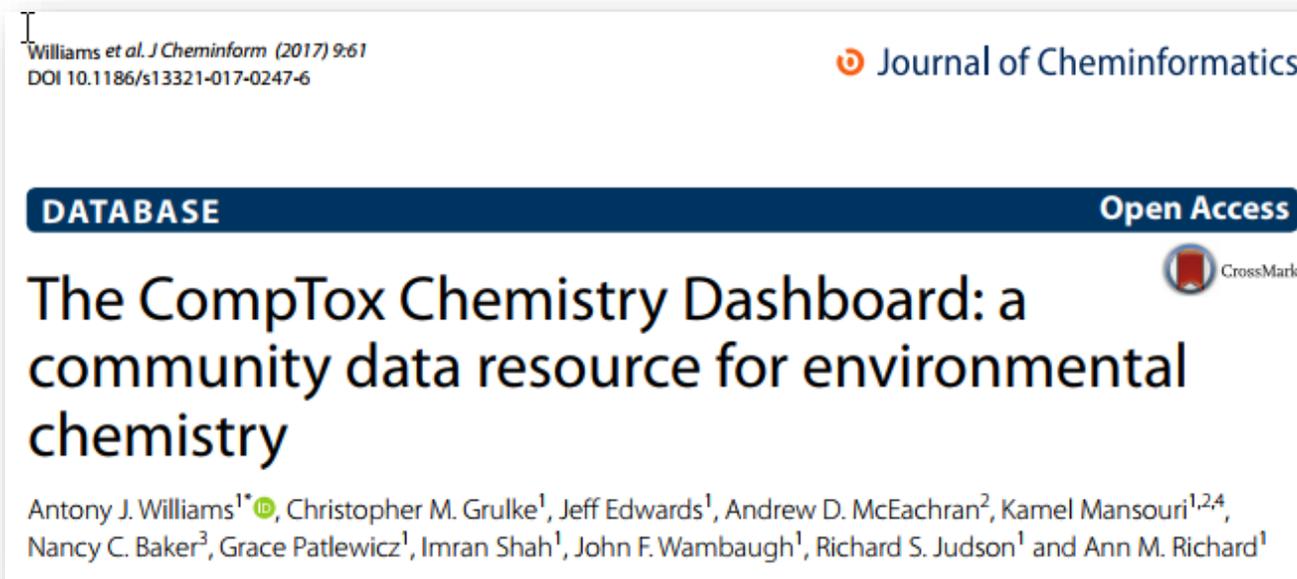
Title	Author	Date
Antony Williams, the ChemConnector: A career path through a diverse series of roles and responsibilities	Antony Williams	09/05/2019
The needs for chemistry standards, database tools and data curation at the chemical-biology interface	Antony Williams, Kamel Mansouri, Ann Richard and Chris Grulke	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	Antony Williams, Manjiv Linsendink, Arvin Crofton, Russell Thomas and Jeffrey Edwards	30/06/2017
Consensus ranking and fragmentation prediction for identification of unknowns in high resolution mass spectrometry	Andrew D. 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, Chris Grulke, Ann Richard, Richard Judson, Arman Shah, Grace Patlewicz, John Wombough, Katie Paul-Friedman, Jeremy Dunne and Jeff Edwards	09/10/2019
Generalised Read-Across GenRA, research, implementation and practical application	Grace Patlewicz	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 J. Williams, Andrew McEachran, Jon Sobus, Seth Newton, Elin Ulrich, Chris Grulke, Kamel Mansouri, Jennifer Smith and Jeff Edwards	30/06/2017

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**DATABASE** **Open Access**

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

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