EPA United States Environmental Protection Agency

EPA Tools and Resources Webinar CompTox Dashboard:

Data and Tools to Support Chemical and Environmental Risk Assessment

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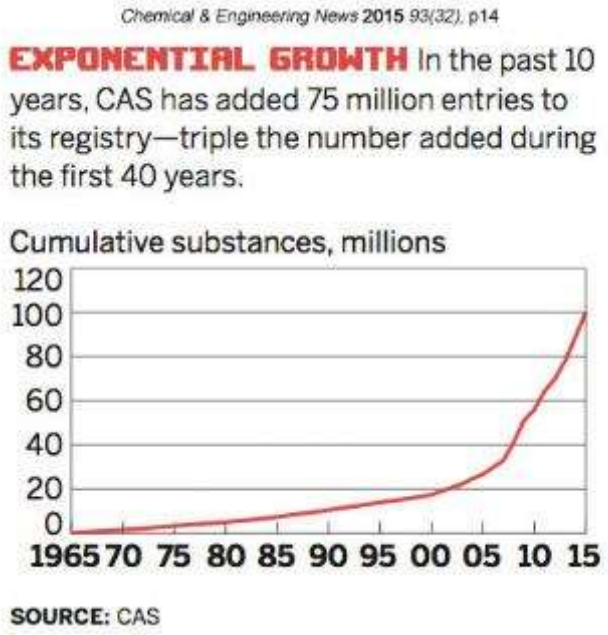
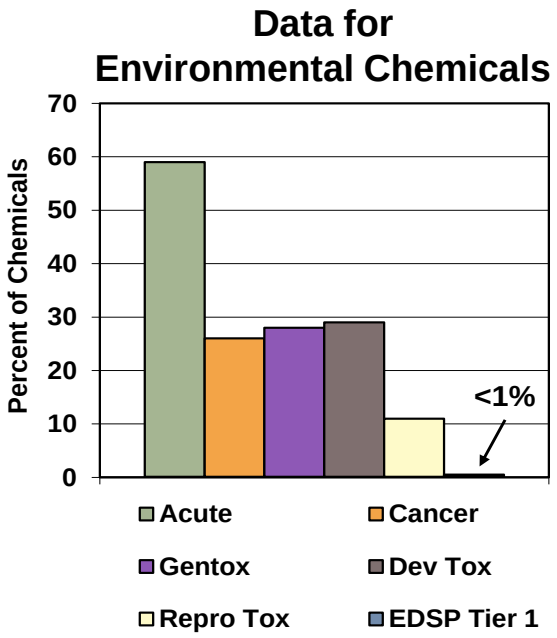
Problem: Too Many Chemicals, too Few Resources

- **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**
  - Significant growth in the number of substances and chemicals / and the associated data
  - Nearly 60% of chemicals on various EPA lists have acute toxicity data, 30% have data on other types of toxicity



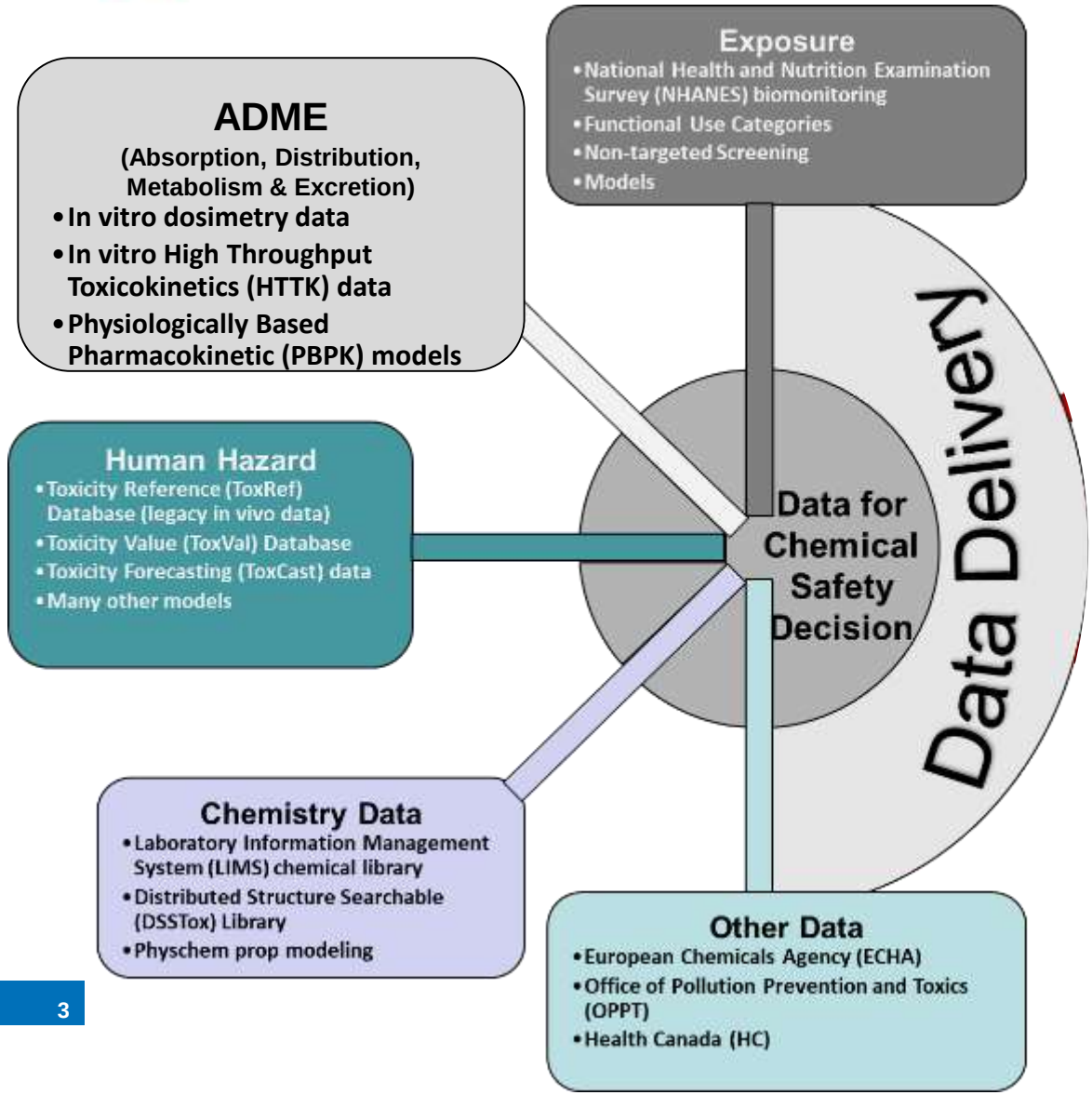


Modified from Judson *et al.*, EHP 2010

Approach

- **Develop a "one-stop-shop" for data as an integration node for environmental chemical data to support EPA and partner decision making:**
  - Centralized location for relevant chemical safety 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**

Approach

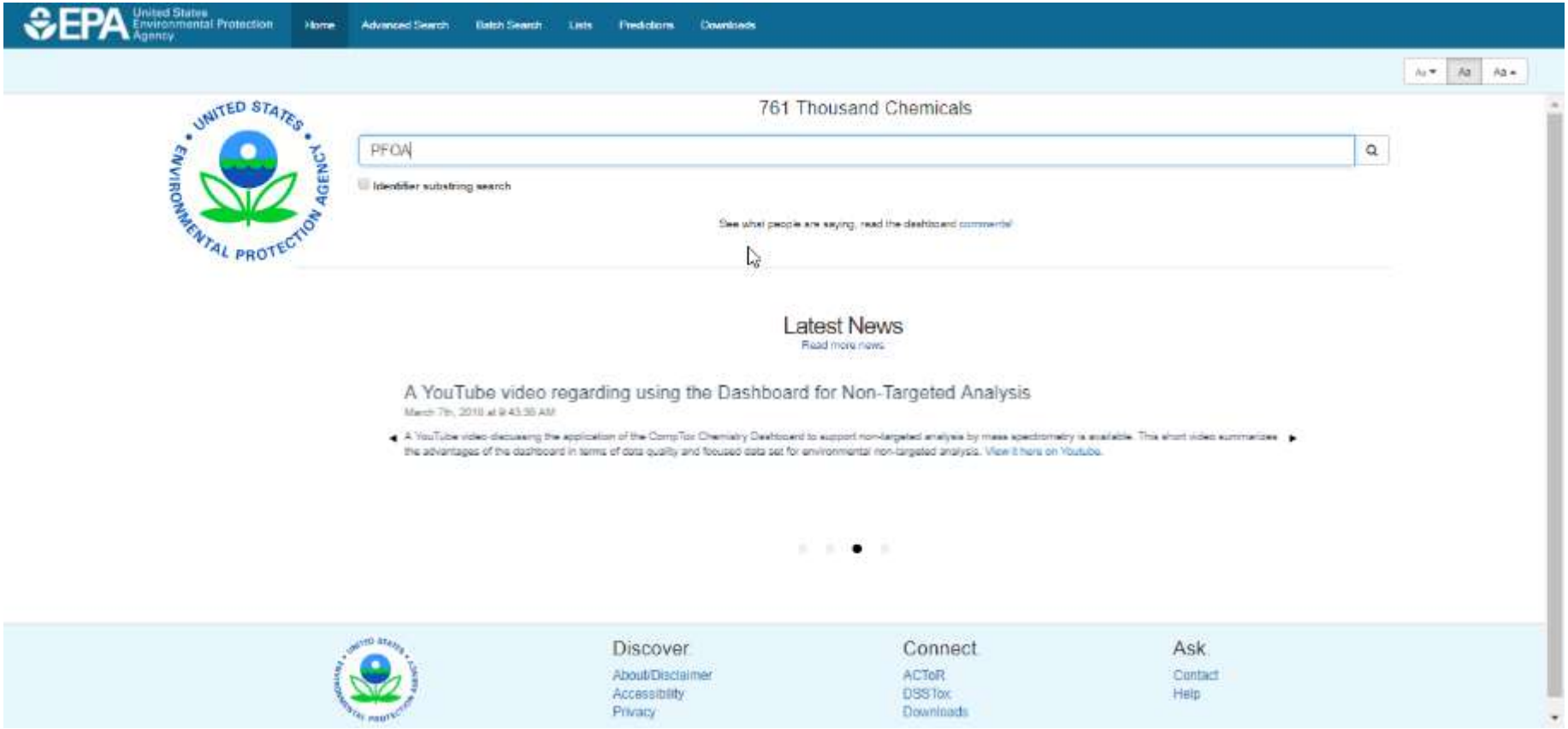

Exposure
•National Health and Nutrition Examination Survey (NHANES) biomonitoring
•Functional Use Categories
•Non-targeted Screening
•Models
ADME
(Absorption, Distribution, Metabolism & Excretion)
•In vitro dosimetry data
•In vitro High Throughput Toxicokinetics (HTTK) data
•Physiologically Based Pharmacokinetic (PBPK) models
Human Hazard
•Toxicity Reference (ToxRef) Database (legacy in vivo data)
•Toxicity Value (ToxVal) Database
•Toxicity Forecasting (ToxCast) data
•Many other models
Data for Chemical Safety Decision
Data Delivery
Chemistry Data
•Laboratory Information Management System (LIMS) chemical library
•Distributed Structure Searchable (DSSTox) Library
•Physchem prop modeling
Other Data
•European Chemicals Agency (ECHA)
•Office of Pollution Prevention and Toxics (OPPT)
•Health Canada (HC)

Results: EPA's CompTox Dashboard

A publicly accessible website delivering:

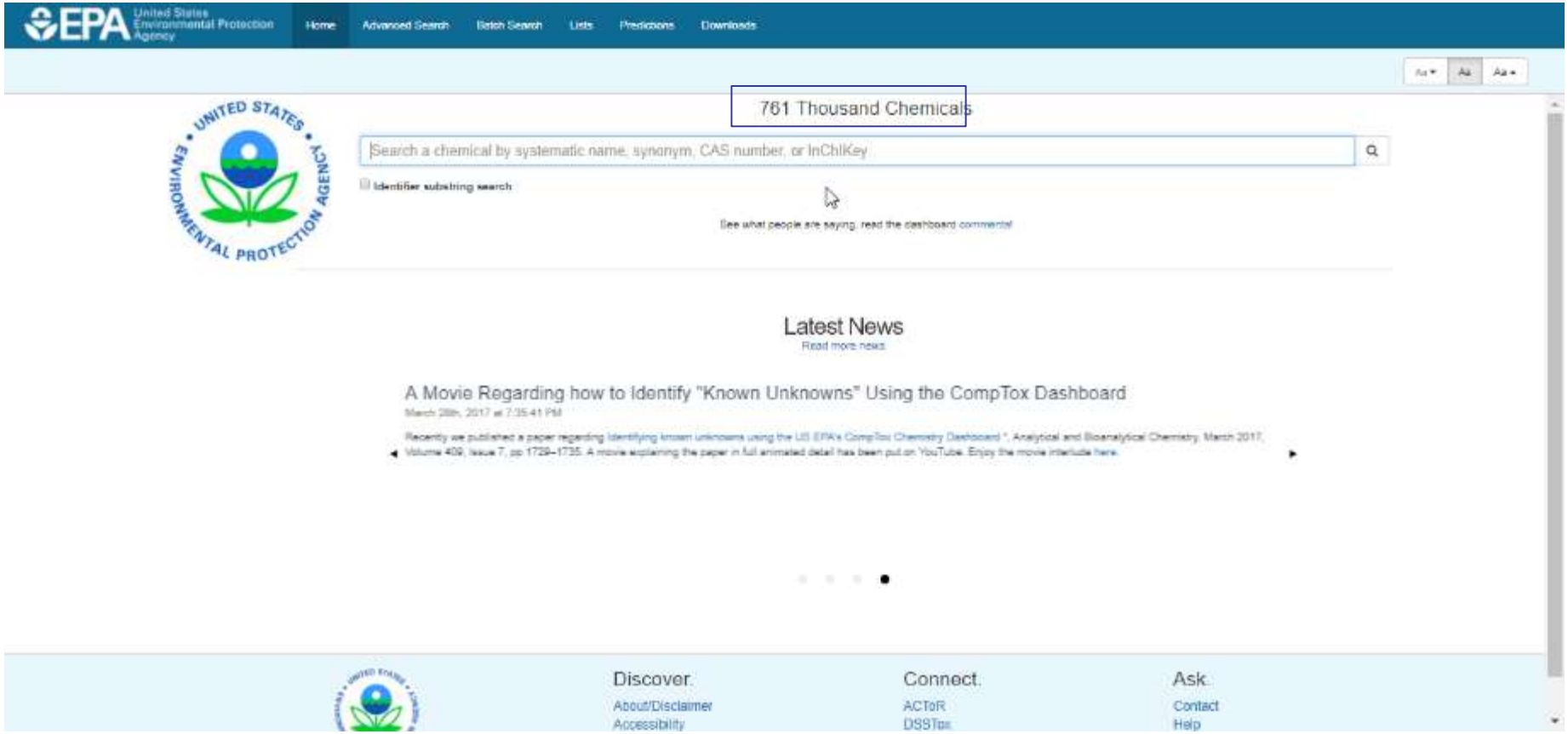
- ~760,000 chemicals with related property data
- Experimental and predicted physicochemical property data
- Integration to "biological assay data" for 1000's of chemicals
- Information regarding consumer products containing chemicals
- Generalized Read-Across (GenRA) module
- Links to other agency websites 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

EPA CompTox Dashboard: Live Demo

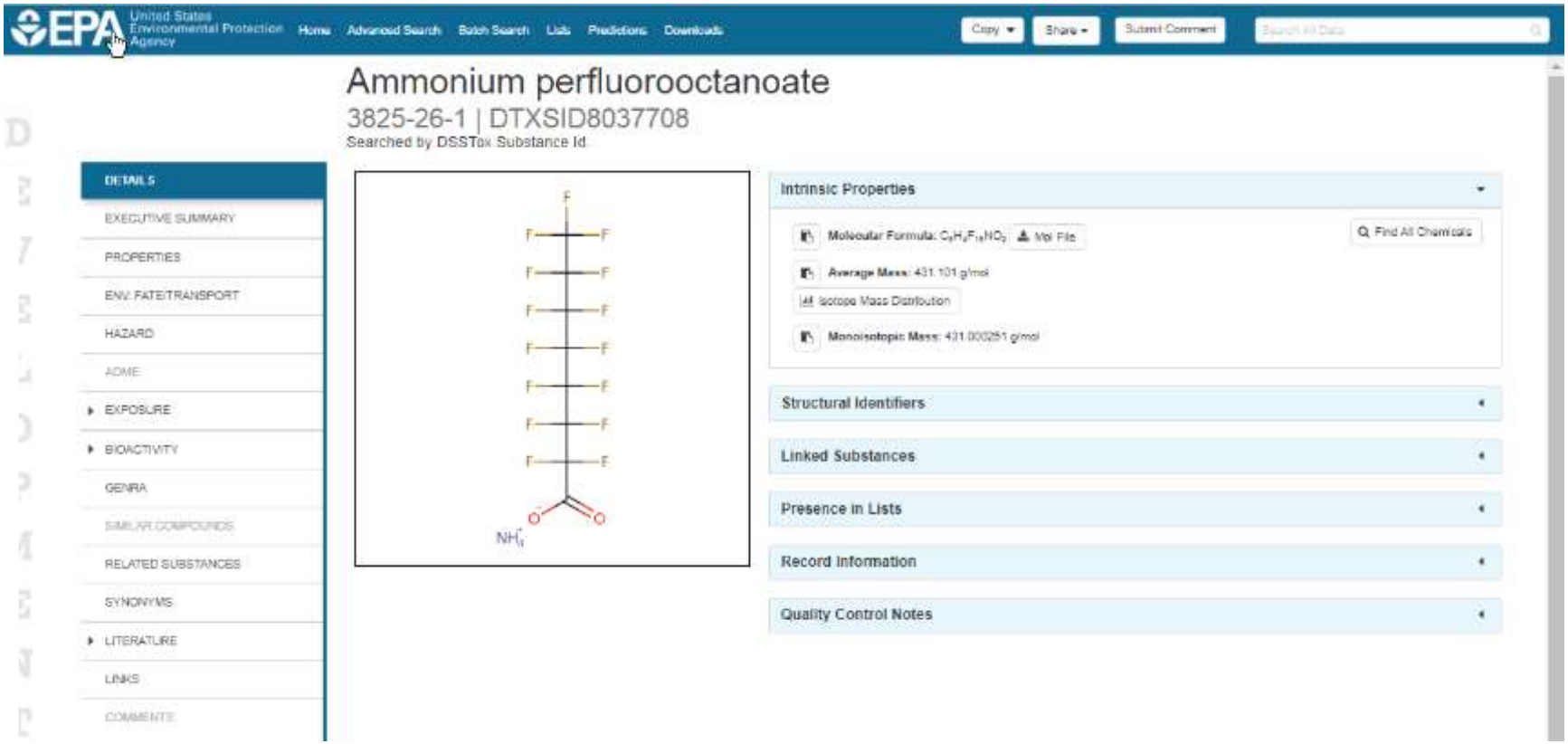


CompTox Dashboard

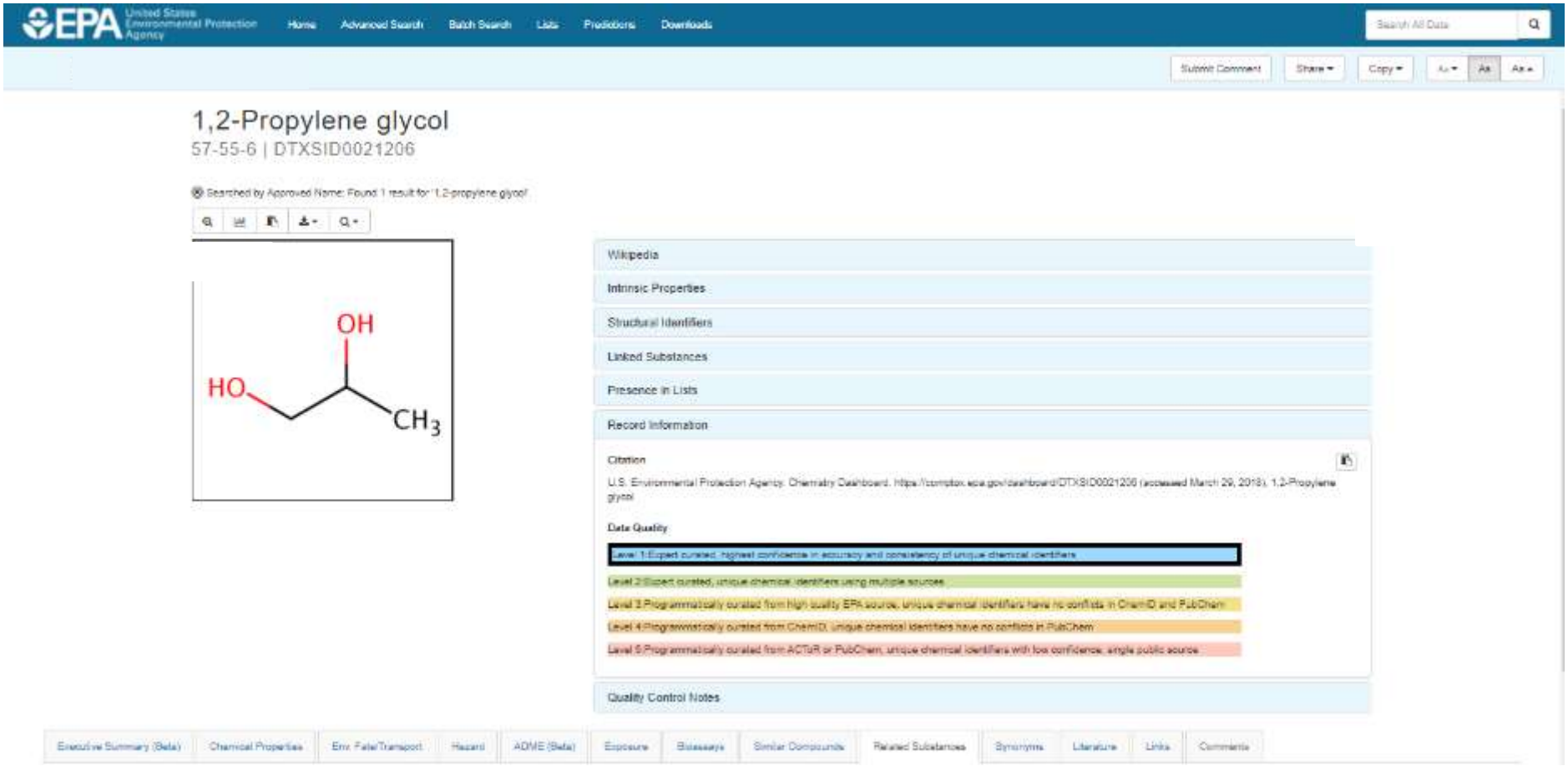
https://comptox.epa.gov/dashboard



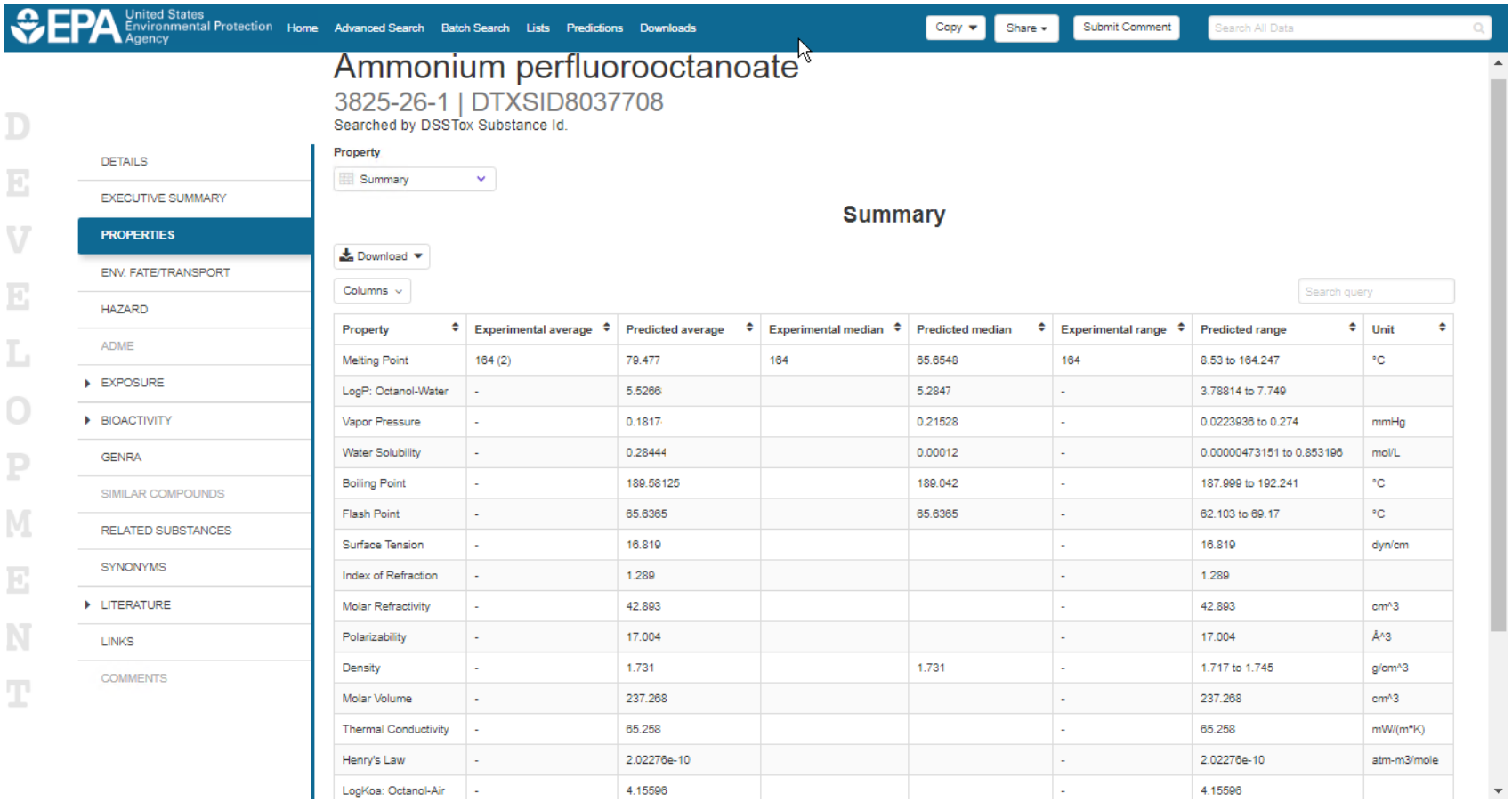
Detailed Chemical Pages



Data Quality

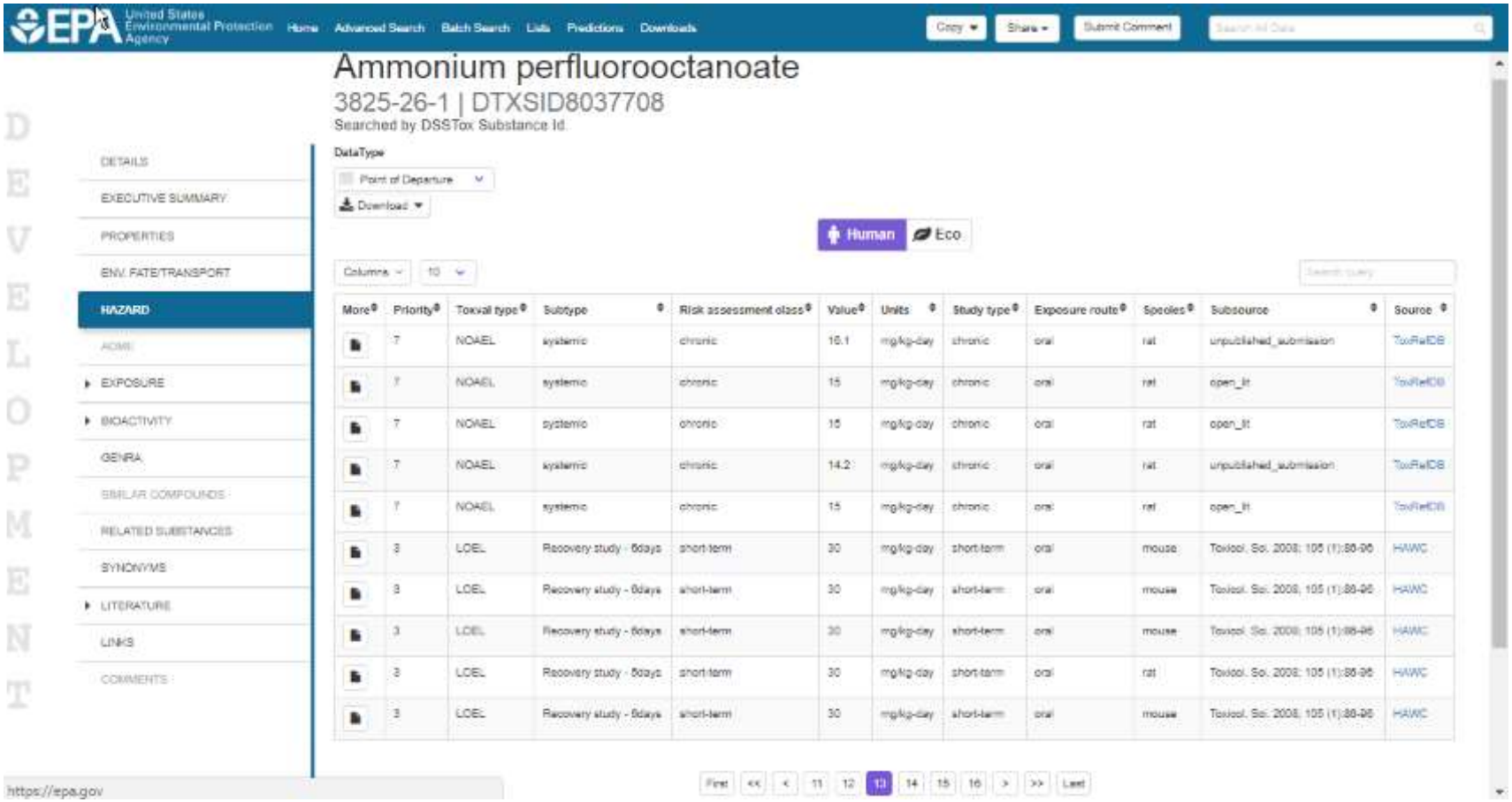


Properties, Fate and Transport



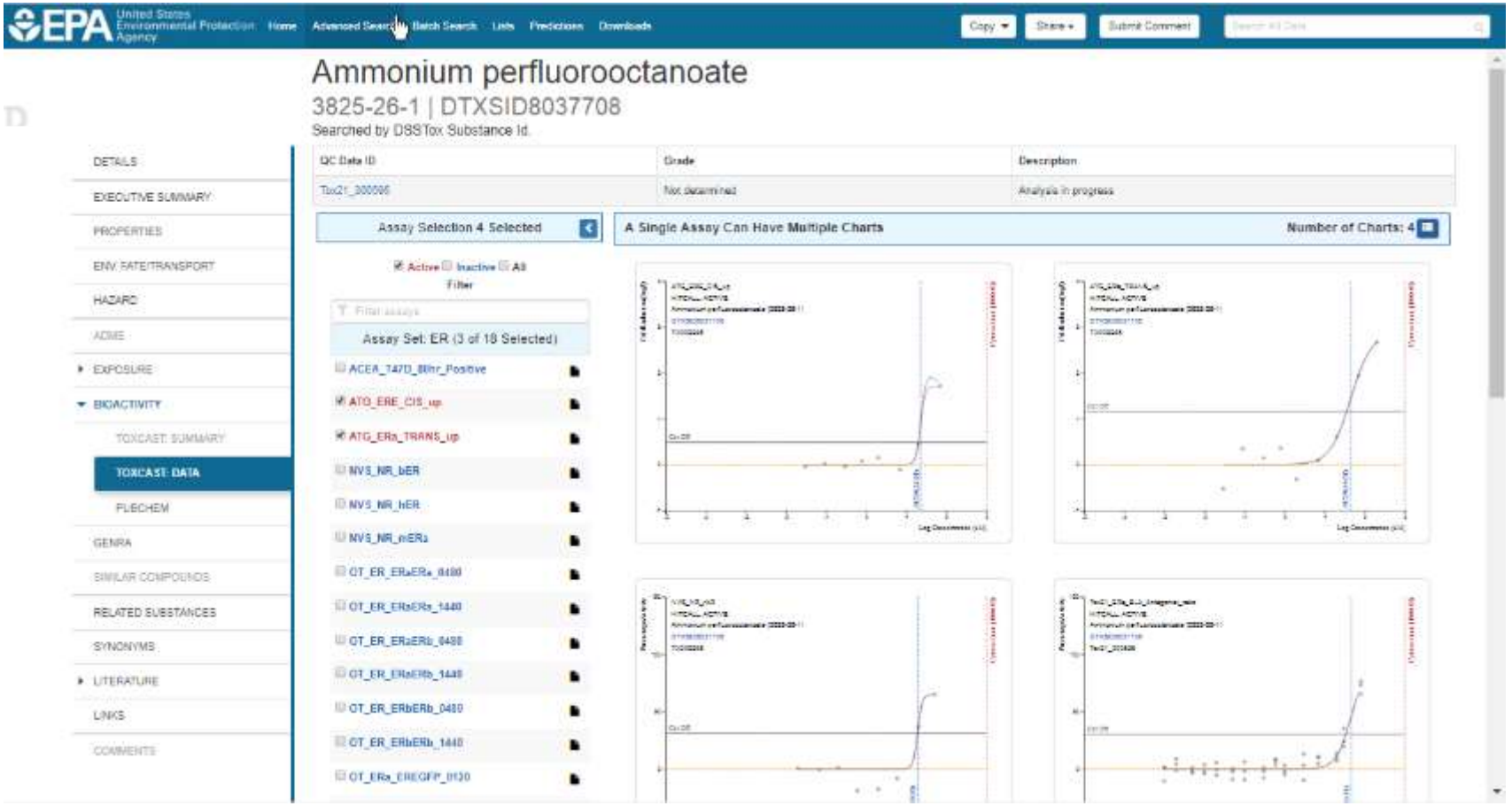
Property	Experimental average	Predicted average	Experimental median	Predicted median	Experimental range	Predicted range	Unit
Melting Point	164 (2)	79.477	164	65.6548	164	8.53 to 164.247	°C
LogP: Octanol-Water	-	5.5266		5.2847	-	3.78814 to 7.749	
Vapor Pressure	-	0.1817		0.21528	-	0.0223936 to 0.274	mmHg
Water Solubility	-	0.28444		0.00012	-	0.00000473151 to 0.853196	mol/L
Boiling Point	-	189.58125		189.042	-	187.999 to 192.241	°C
Flash Point	-	65.6365		65.6365	-	62.103 to 69.17	°C
Surface Tension	-	16.819			-	16.819	dyn/cm
Index of Refraction	-	1.289			-	1.289	
Molar Refractivity	-	42.893			-	42.893	cm^3
Polarizability	-	17.004			-	17.004	Å^3
Density	-	1.731		1.731	-	1.717 to 1.745	g/cm^3
Molar Volume	-	237.268			-	237.268	cm^3
Thermal Conductivity	-	65.258			-	65.258	mW/(m*K)
Henry's Law	-	2.02276e-10			-	2.02276e-10	atm-m3/mole
LogKoa: Octanol-Air	-	4.15596			-	4.15596	

Chemical Hazard Data

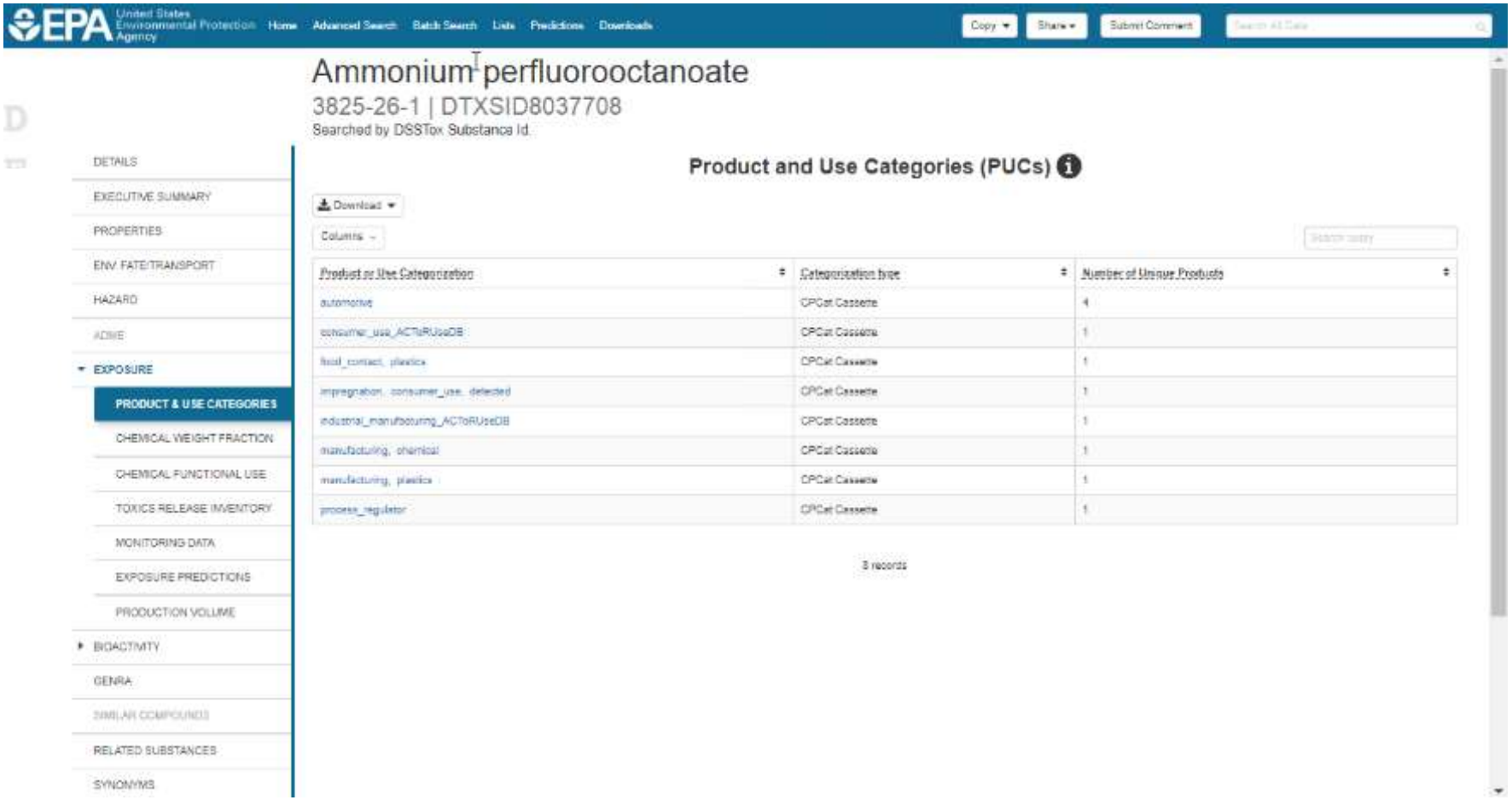


In Vitro Bioassay Screening

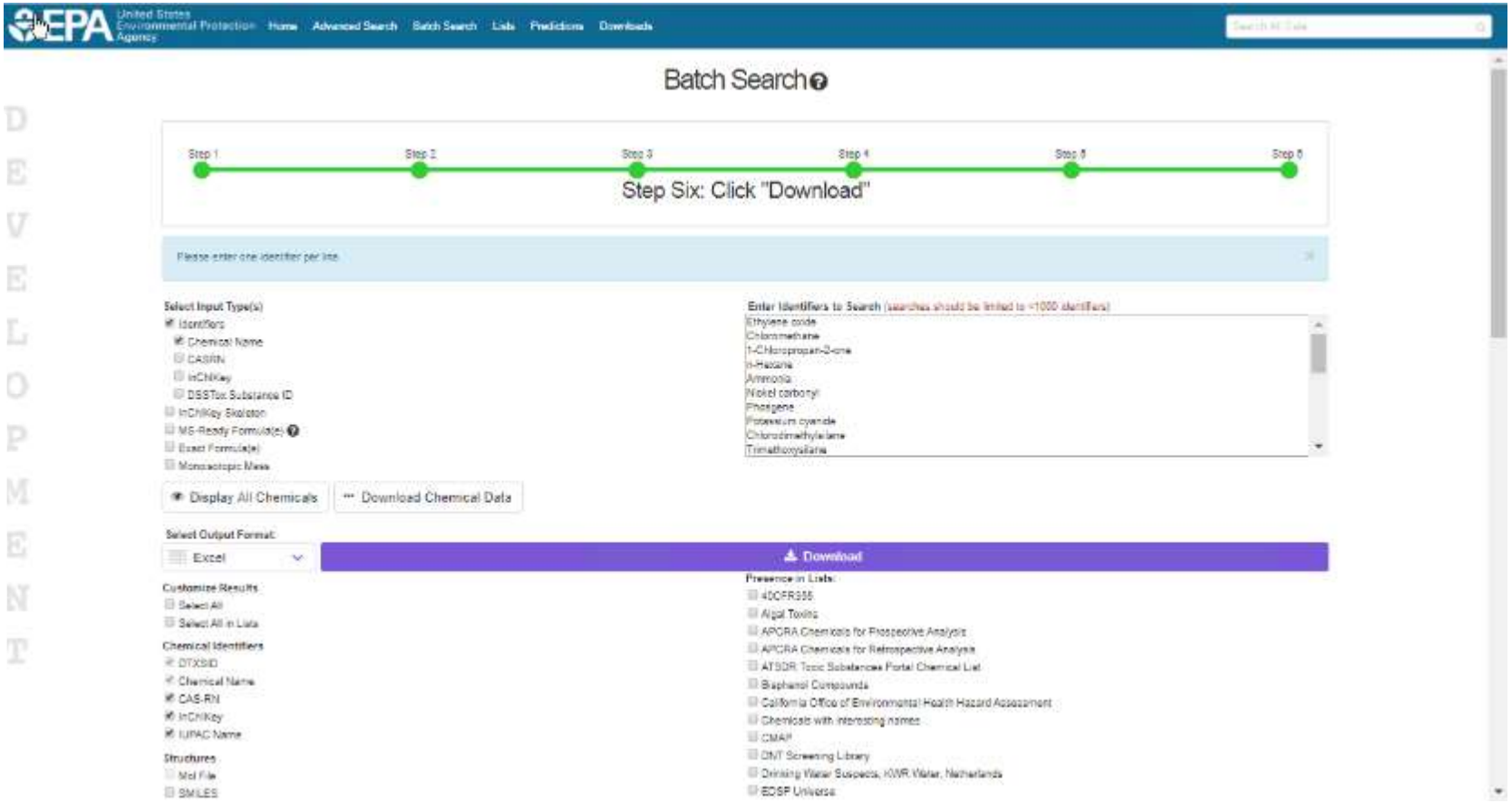
ToxCast and Tox21



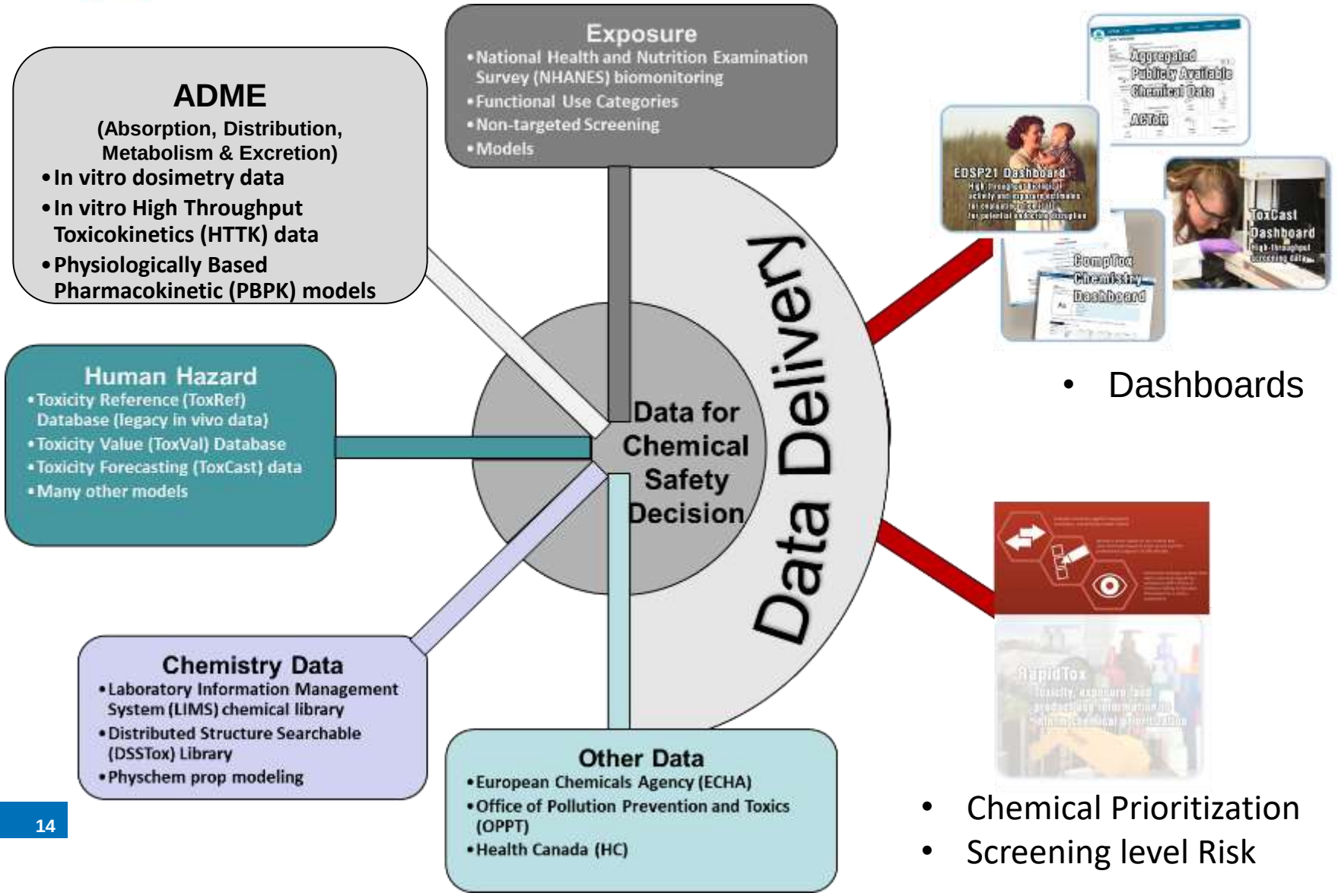
Sources of Exposure to Chemicals



Searching for more than one Chemical: Batch Searching



Impact



- Dashboards

- Chemical Prioritization
- Screening level Risk

Impact

- An integration hub for multiple “modules”
  - Experimental and predicted properties
  - Human and Ecological Hazard data
  - Exposure data – products, data in the environment
  - *In vitro* bioassay data – ToxCast/Tox21
  - Literature searching – Google Scholar and PubMed
  - Specialized searches – mass/formula for analytical support
  - Batch searching and Real Time Predictions
- CompTox Dashboard integrates chemical data
- Used by EPA and others to support chemical safety decisions
  - EPA examples: Endocrine Disruptor Screening Program in the 21st Century (EDSP21), Future (RapidTox)

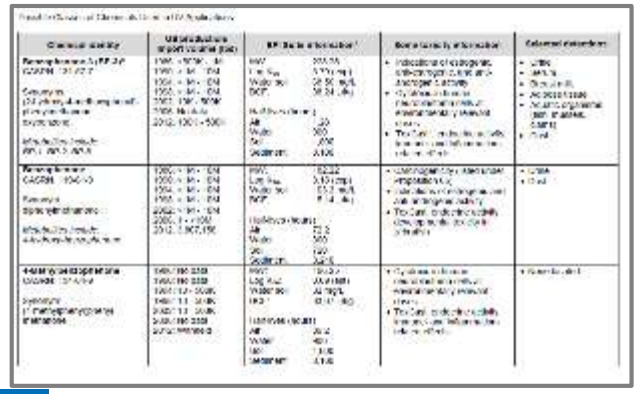
Impact

United States Environmental Protection Agency

Minnesota Dept Health Risk Assessments for Water Contaminant

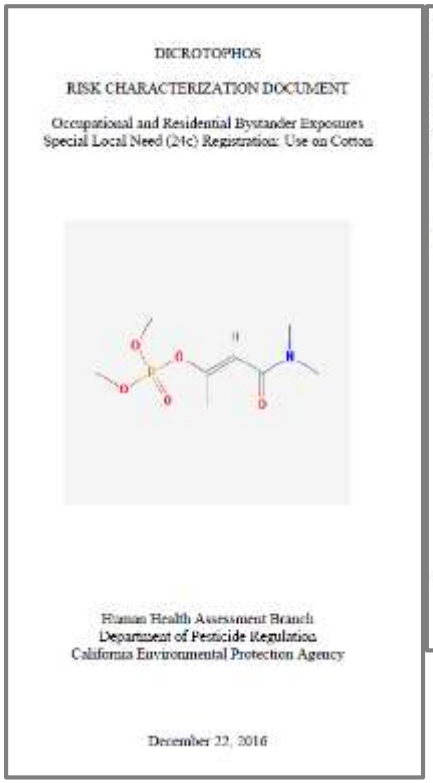
- Pilot study to utilize ToxCast data in Drinking Water Contaminants of Emerging Concern

Prioritization for Biomonitoring CA



- Data surfaced through the EPA CompTox Dashboard utilized to prioritize biomonitoring for of emerging contaminants

CalEPA Pesticide Assessments


DICROTOPHOS

RISK CHARACTERIZATION DOCUMENT

Occupational and Residential Bystander Exposures
Special Local Need (24c) Registration: Use on Cotton

Human Health Assessment Branch
Department of Pesticide Regulation
California Environmental Protection Agency

December 22, 2016

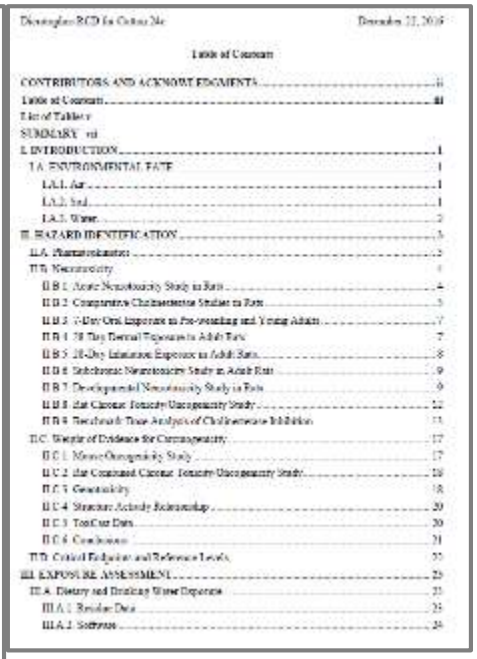


Table of Contents

- ToxCast data used for weight of evidence decisions regarding health effects for pesticides

*Not a comprehensive list

Conclusion

- EPA's CompTox Dashboard provides access to data for ~760,000 chemicals
- High quality data from ongoing curation efforts
- An integration hub for multiple "modules" and tools to support multiple environmental applications
- Major Update to EPA CompTox Dashboard released in August 2018
  - Endocrine Disrupting Compounds (EDCs)
  - Per- and Polyfluoroalkyl Substances (PFAS)
  - Generalized **Read-Across** (GenRA) module

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