The Chemical and Products Database (CPDat)

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National Exposure Research Laboratory

Computational Toxicology Communities of Practice
October 25, 2018

United States Environmental Protection Agency

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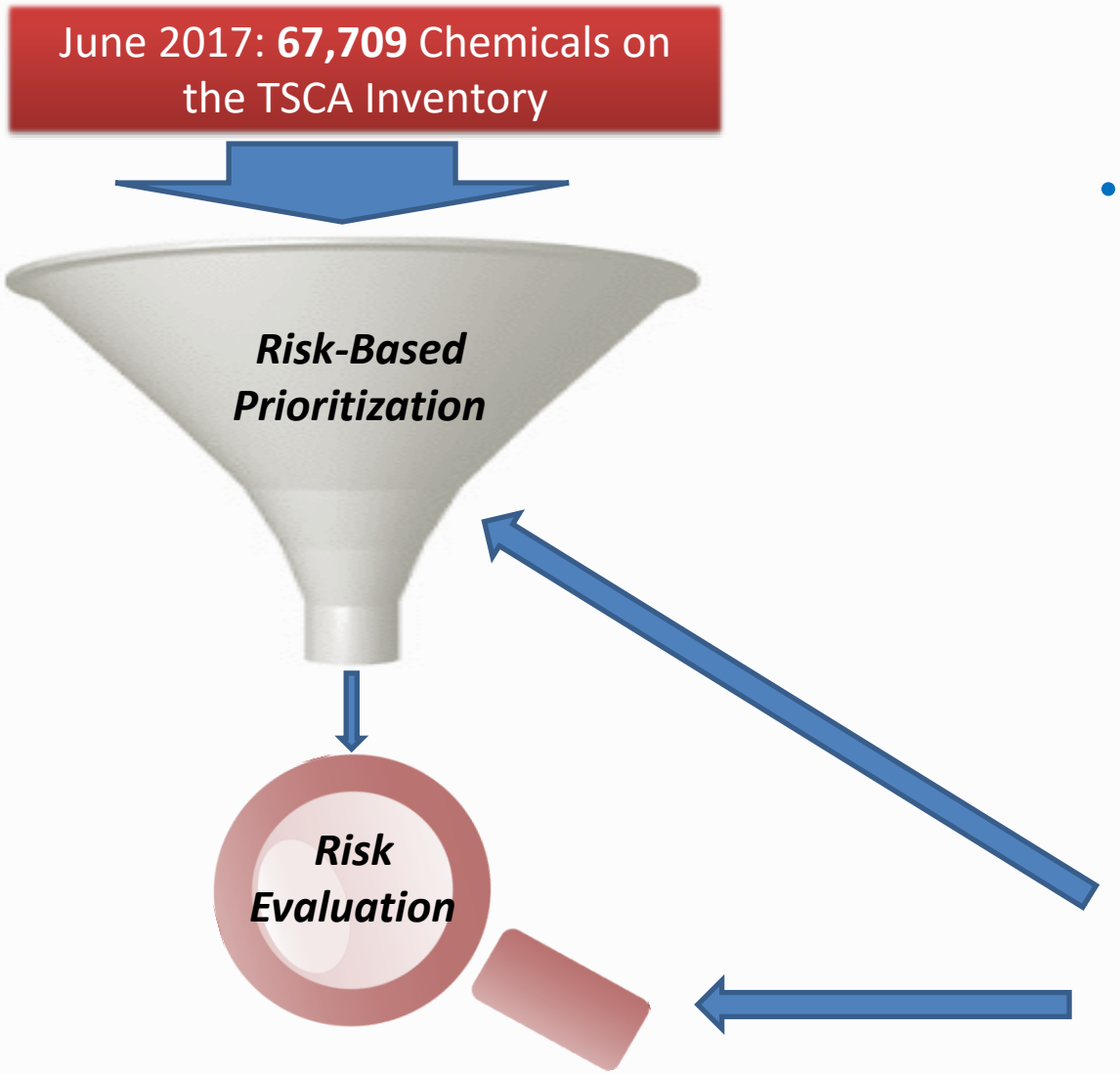
TSCA and the need for exposure information



Frank R. Lautenberg Chemical Safety for the 21st Century Act (June 2016)

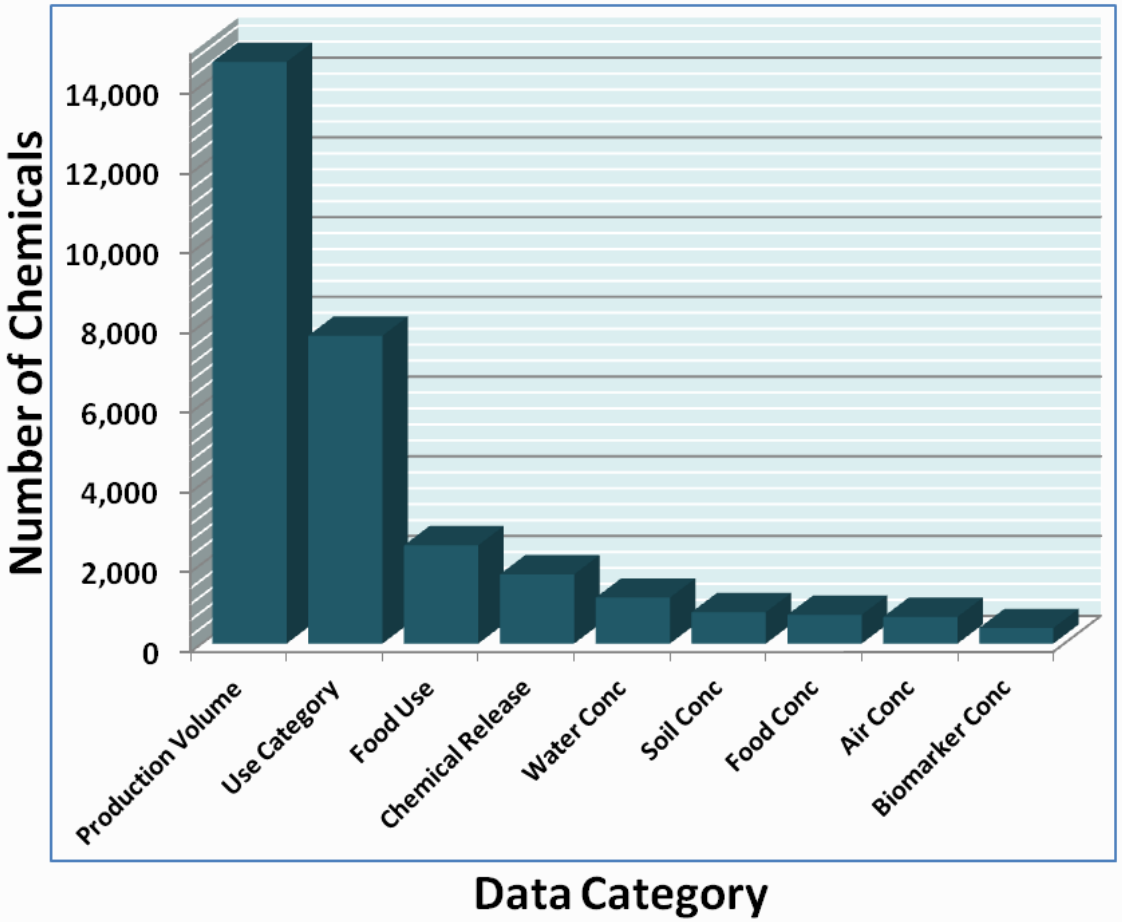
- Amends the Toxic Substances Control Act (TSCA)
  - Mandatory requirement for EPA to evaluate existing chemicals with clear and enforceable deadlines
  - Risk-based chemical assessments
  - Increased public transparency for chemical information

TSCA section 6(b)(1)(A)

- Exposure potential of the chemical substance

Data critical to exposure estimation are limited

67,709 chemicals on the TSCA inventory



Egeghy et al. *Science of the Total Environment* (2012)

Data critical to exposure estimation are limited

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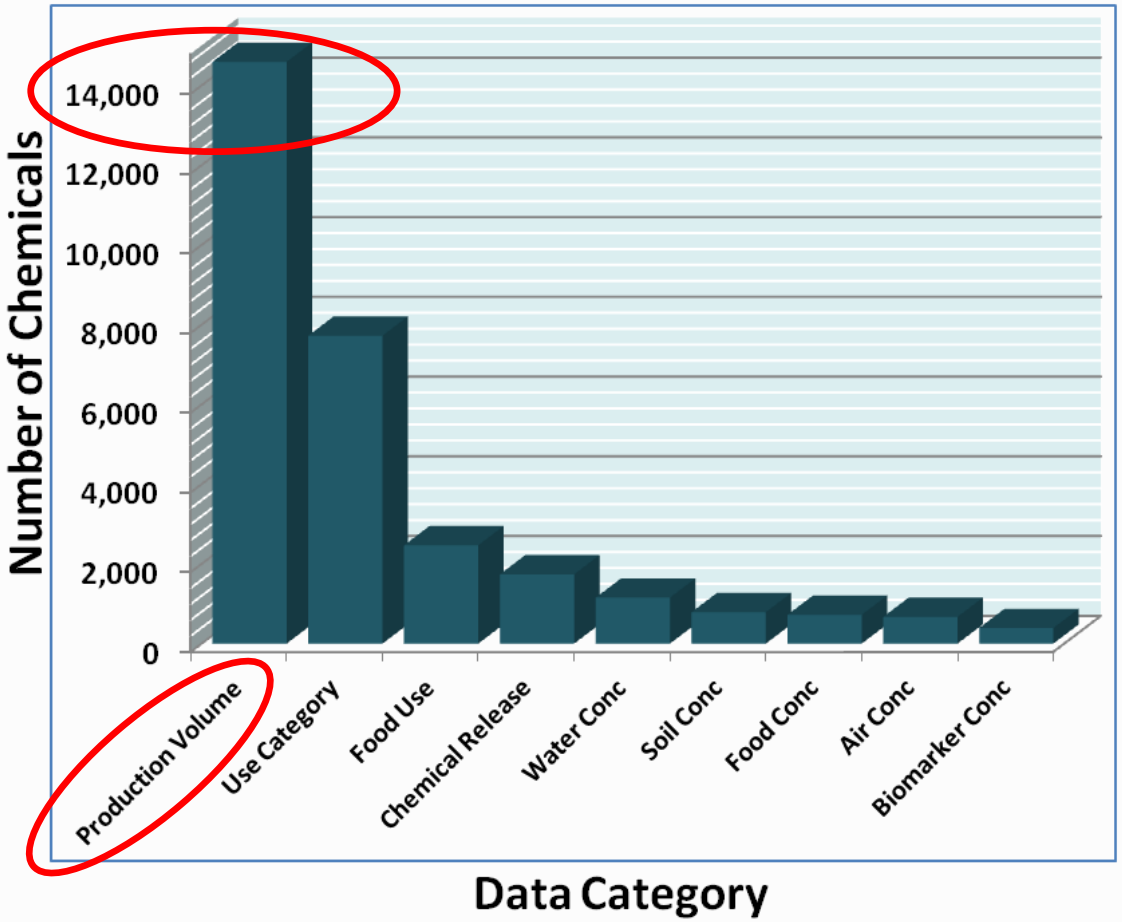

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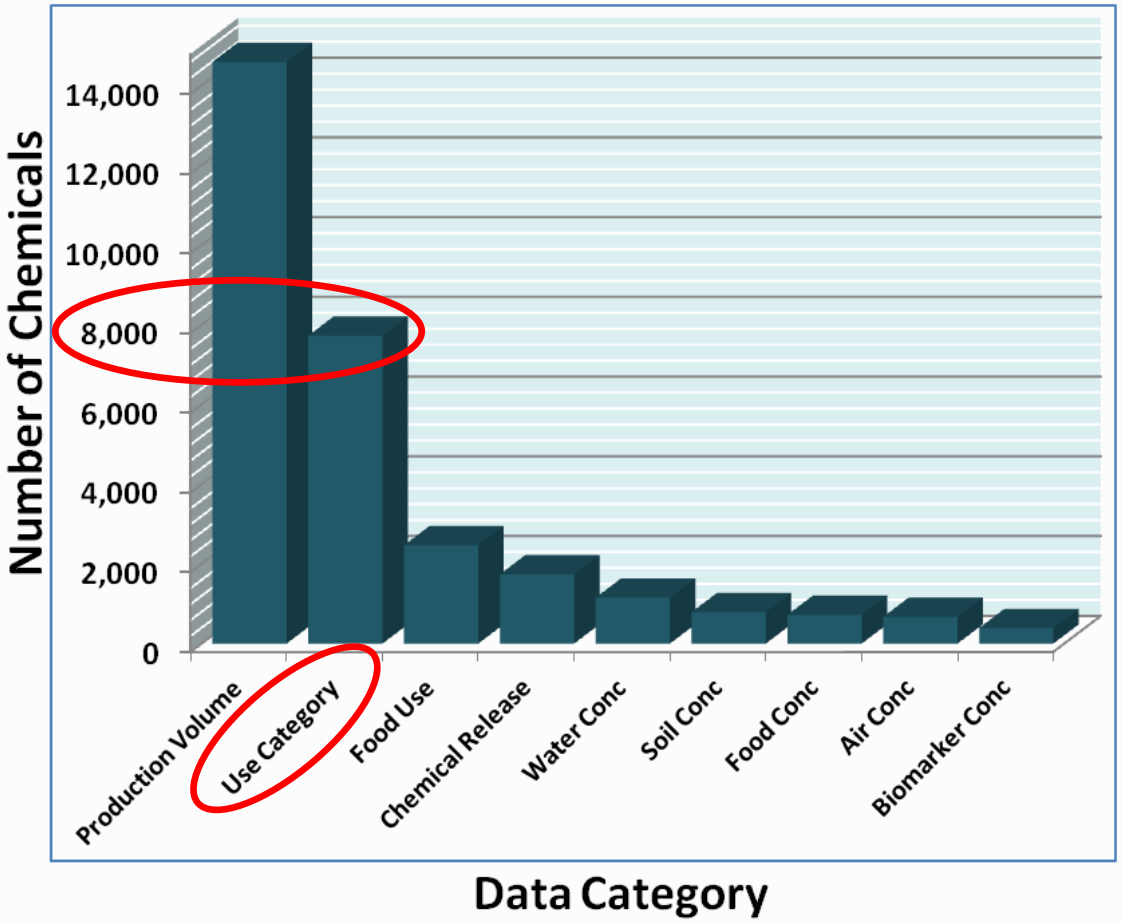


Egeghy et al. *Science of the Total Environment* (2012)

The Chemicals and Products Database (CPDat)

- Information on generic chemical use and the chemical composition of consumer products is needed to support modeling-based characterization of population chemical exposures
  - Existing data is widely dispersed and difficult to access
  - Data from multiple EPA efforts need to be harmonized and organized
  - Data are needed on why a chemical is in a product
- EPA has collected data from multiple sources and consolidated them into an integrated relational database of *chemical* and *consumer product* information:

CPDat
Chemical and Products Database

CompTox Dashboard

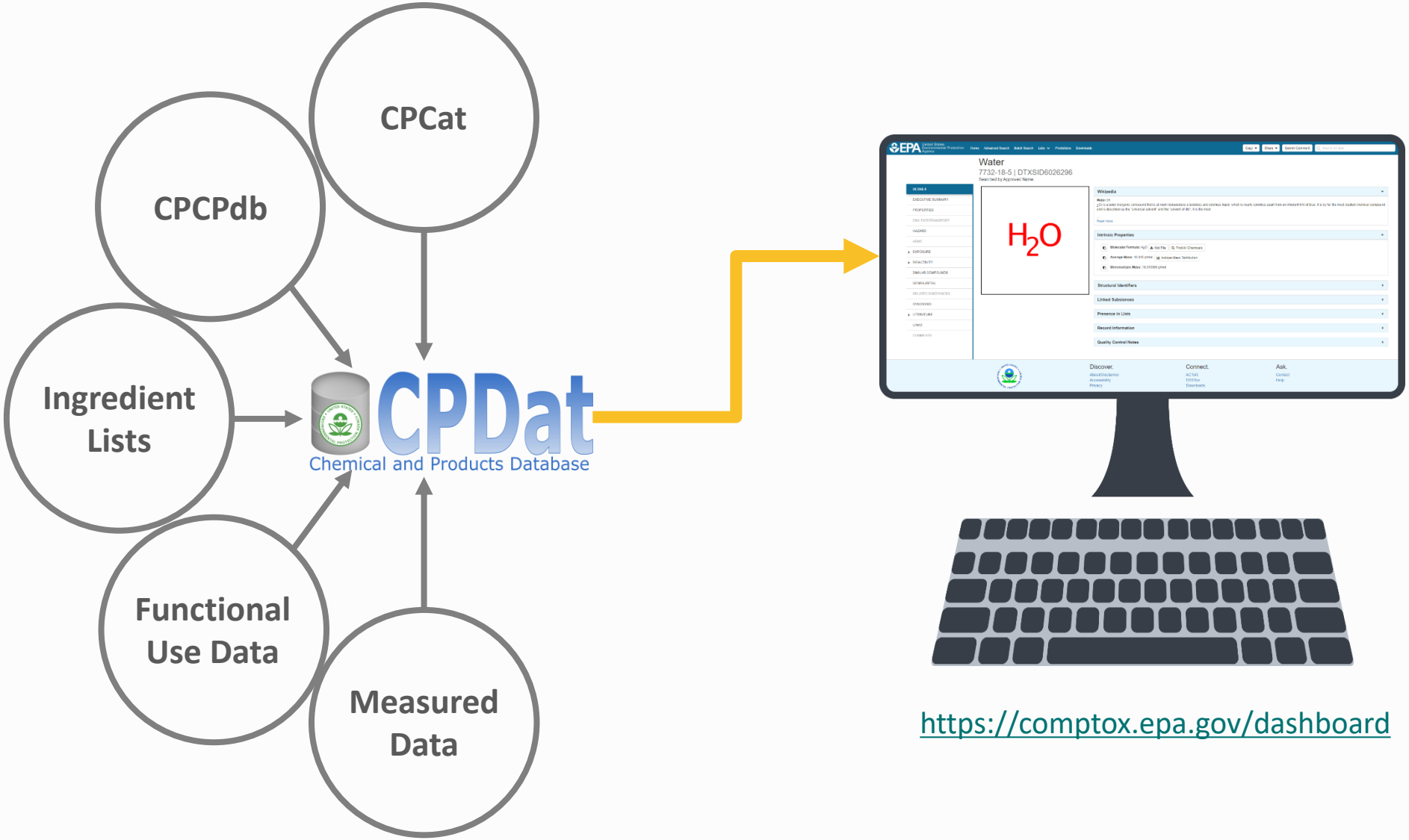
The Chemicals and Products Database (CPDat)

- Provides a means to organize and disseminate chemical and product information
- Comprised of chemical use and consumer product composition data from a variety of public sources; includes measured, modeled, and reported data
- Organized around a set of consumer product use categories (PUCs) optimized for exposure modeling
- Incorporating exposure from near-field sources into health characterization for risk-based prioritization
- Sustainable way to ***organize, update, and disseminate these data***

CPDat
Chemical and Products Database

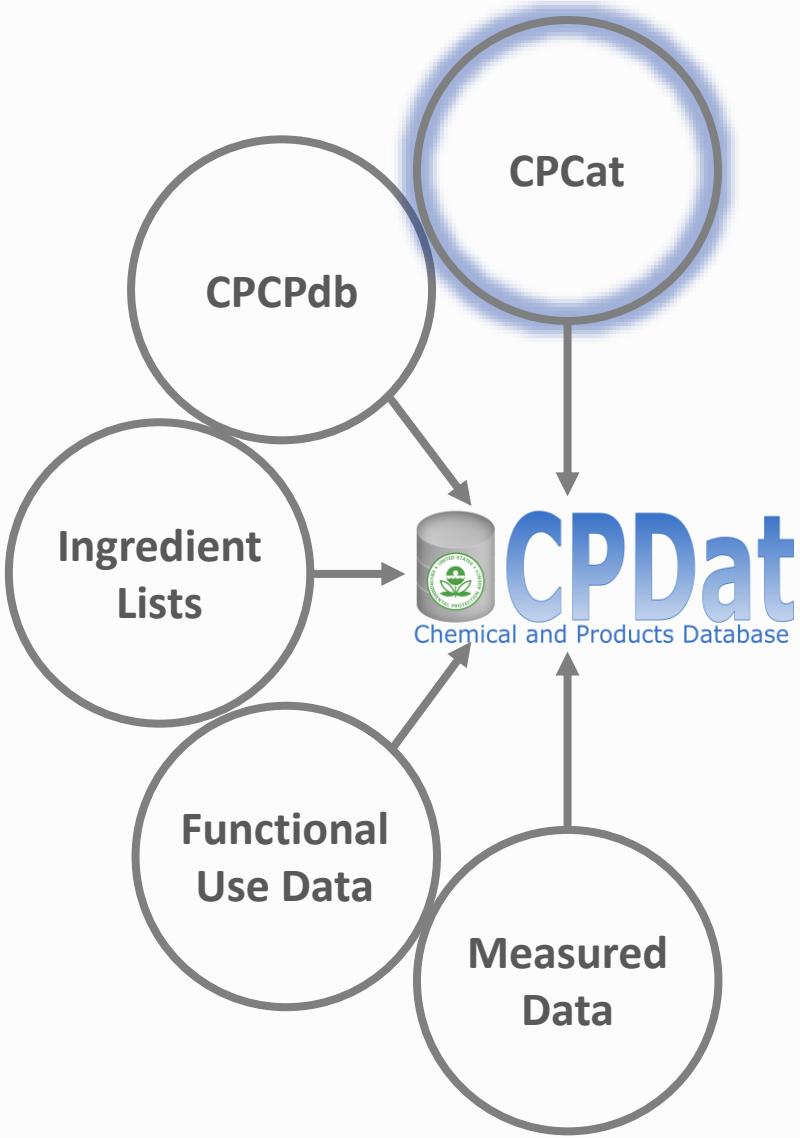
CompTox Dashboard

What is CPDat?



https://comptox.epa.gov/dashboard

What is CPDat?



Contents lists available at ScienceDirect

Toxicology Reports

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

Exploring consumer exposure pathways and patterns of use for chemicals in the environment

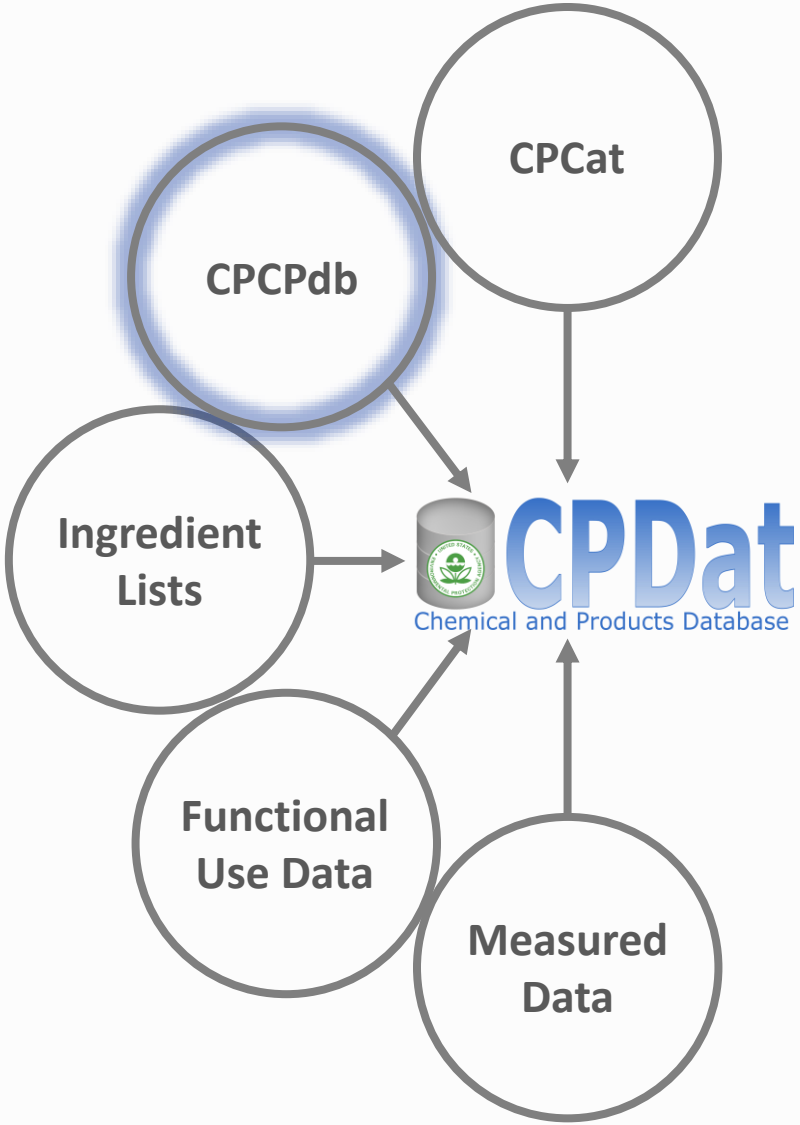
Kathie L. Dionisio[a], Alicia M. Frame[b,1], Michael-Rock Goldsmith[a,2], John F. Wambaugh[b], Alan Liddell[c,3], Tommy Cathey[d], Doris Smith[b], James Vail[b], Alexi S. Ernstoff[e], Peter Fantke[e], Olivier Jolliet[f], Richard S. Judson[b,*]

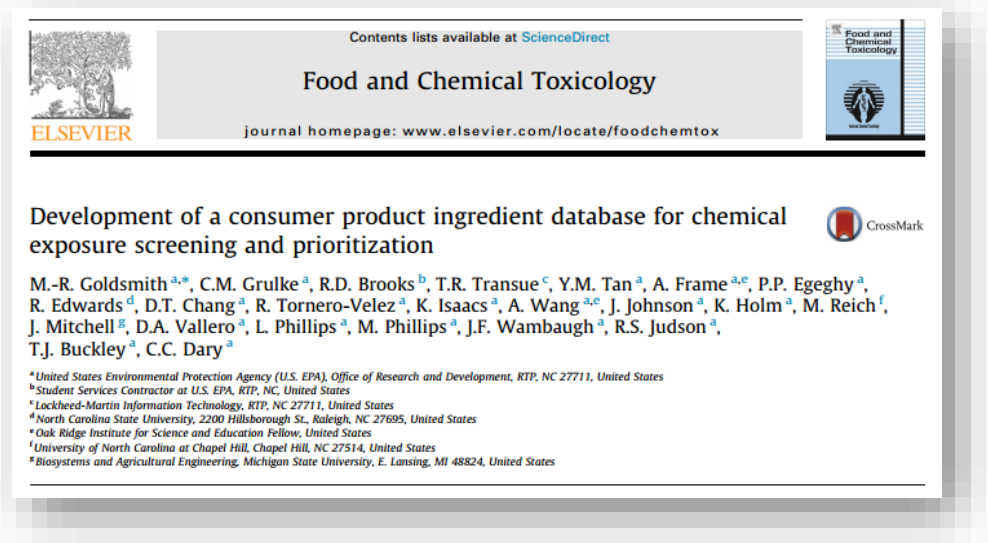
[a] U.S. Environmental Protection Agency, National Exposure Research Laboratory, 109 T.W. Alexander Drive, MC E205-02, Research Triangle Park, NC 27709, USA
[b] U.S. Environmental Protection Agency, National Center for Computational Toxicology, MC B205-01, Research Triangle Park, NC 27709, USA
[c] North Carolina State University, Department of Mathematics, Box 8205, Raleigh, NC 27695-8205, USA
[d] Lockheed Martin, Research Triangle Park, NC, USA
[e] Quantitative Sustainability Assessment, Department of Management Engineering, Technical University of Denmark, Produktionstorvet 424, 2800 Kgs. Lyngby, Denmark
[f] Department of Environmental Health Sciences, School of Public Health, University of Michigan, 1415 Washington Heights, Ann Arbor, MI 48109, USA

Broad categorization of chemical use

- Functional use
- Therapeutic use
- Consumer product-based use
- Industrial process use

What is CPDat?





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Food and Chemical Toxicology

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

Development of a consumer product ingredient database for chemical exposure screening and prioritization

M.-R. Goldsmith [a,*], C.M. Grulke [a], R.D. Brooks [b], T.R. Transue [c], Y.M. Tan [a], A. Frame [a,e], P.P. Egeghy [a], R. Edwards [d], D.T. Chang [a], R. Tornero-Velez [a], K. Isaacs [a], A. Wang [a,e], J. Johnson [a], K. Holm [a], M. Reich [f], J. Mitchell [g], D.A. Vallero [a], L. Phillips [a], M. Phillips [a], J.F. Wambaugh [a], R.S. Judson [a], T.J. Buckley [a], C.C. Dary [a]

[a] United States Environmental Protection Agency (U.S. EPA), Office of Research and Development, RTP, NC 27711, United States
[b] Student Services Contractor at U.S. EPA, RTP, NC, United States
[c] Lockheed-Martin Information Technology, RTP, NC 27711, United States
[d] North Carolina State University, 2200 Hillsborough St., Raleigh, NC 27695, United States
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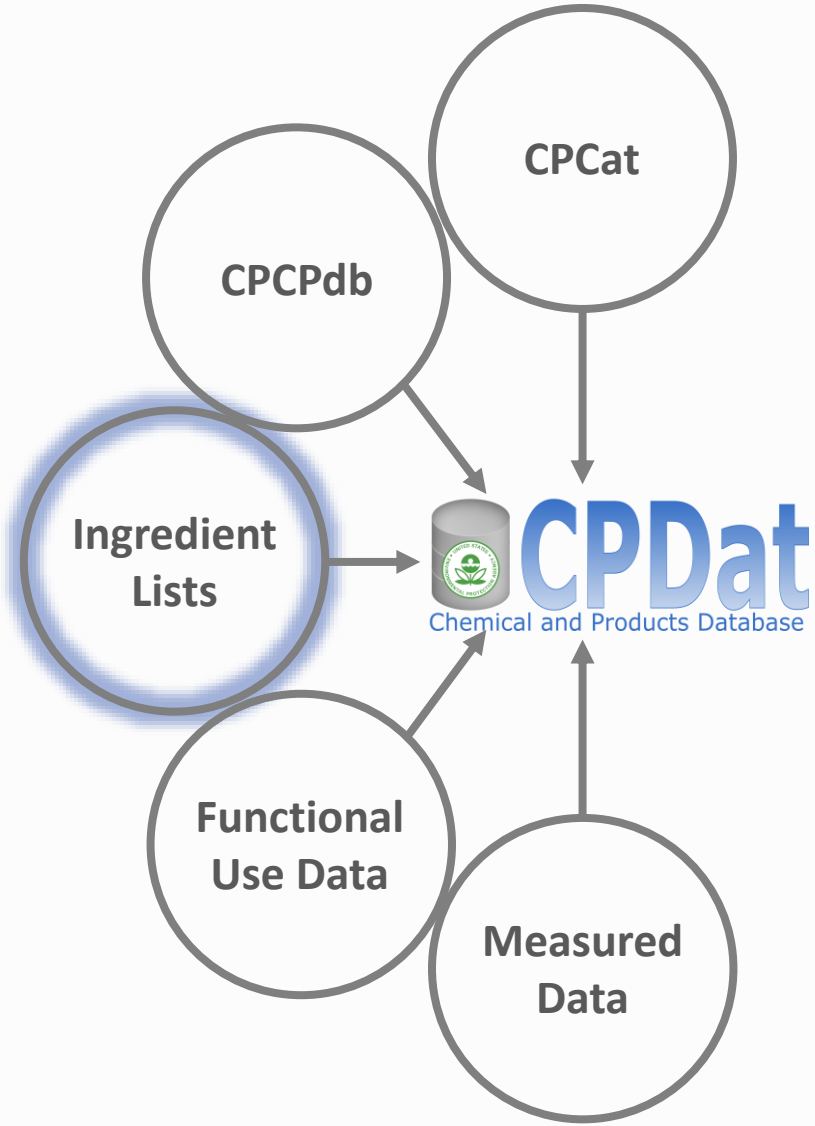
[f] University of North Carolina at Chapel Hill, Chapel Hill, NC 27514, United States
[g] Biosystems and Agricultural Engineering, Michigan State University, E. Lansing, MI 48824, United States

MSDS-based composition information for consumer product formulations

- Includes range of reported weight fraction
- Provides quantitative input to consumer exposure models

What is CPDat?



Journal of Exposure Science and Environmental Epidemiology (2017) 00, 1–7

www.nature.com/jes

ORIGINAL ARTICLE

Consumer product chemical weight fractions from ingredient lists

Kristin K. Isaacs[1], Katherine A. Phillips[1], Derya Biryol[1,2], Kathie L. Dionisio[1] and Paul S. Price[1]

Assessing human exposures to chemicals in consumer products requires composition information. However, comprehensive composition data for products in commerce are not generally available. Many consumer products have reported ingredient lists that are constructed using specific guidelines. A probabilistic model was developed to estimate quantitative weight fraction (WF) values that are consistent with the rank of an ingredient in the list, the number of reported ingredients, and labeling rules. The model provides the mean, median, and 95% upper and lower confidence limit WFs for ingredients of any rank in lists of any length. WFs predicted by the model compared favorably with those reported on Material Safety Data Sheets. Predictions for chemicals known to provide specific functions in products were also found to reasonably agree with reported WFs. The model was applied to a selection of publicly available ingredient lists, thereby estimating WFs for 1293 unique ingredients in 1123 products in 81 product categories. Predicted WFs, although less precise than reported values, can be estimated for large numbers of product–chemical combinations and thus provide a useful source of data for high-throughput or screening-level exposure assessments.

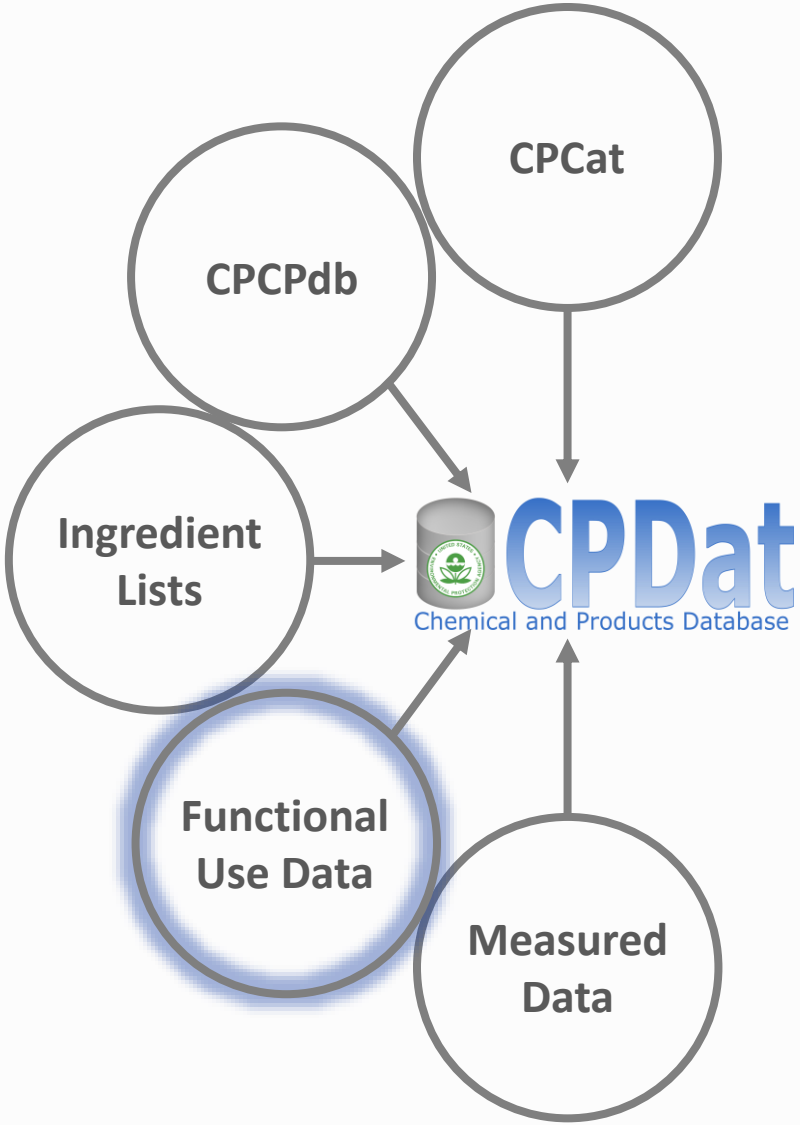
Journal of Exposure Science and Environmental Epidemiology advance online publication, 8 November 2017; doi:10.1038/jes.2017.29

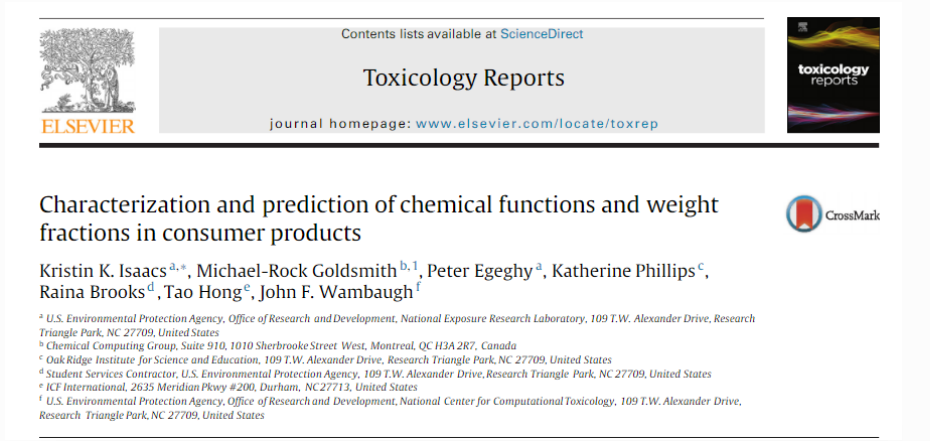
Keywords: consumer products; consumer exposures; ExpoCast; ingredients

Chemical composition of consumer products from ingredient lists

- Reported ingredients
- Predicted weight fractions based on structured reporting rules

What is CPDat?




Contents lists available at ScienceDirect

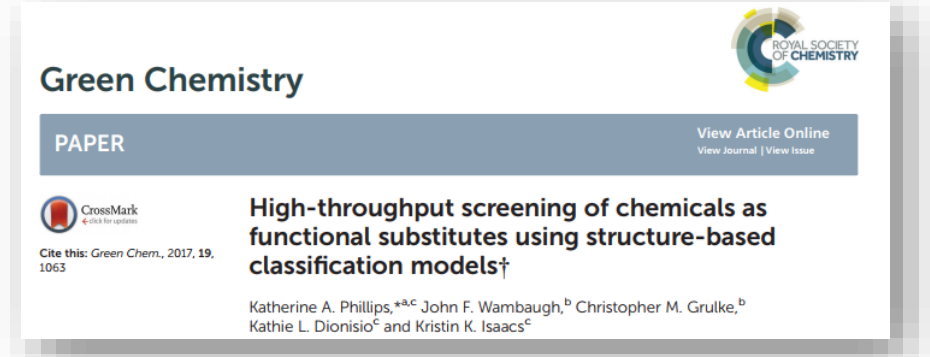
Toxicology Reports

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

Characterization and prediction of chemical functions and weight fractions in consumer products

Kristin K. Isaacs[a,*], Michael-Rock Goldsmith[b,1], Peter Egeghy[a], Katherine Phillips[c], Raina Brooks[d], Tao Hong[e], John F. Wambaugh[f]

[a] U.S. Environmental Protection Agency, Office of Research and Development, National Exposure Research Laboratory, 109 T.W. Alexander Drive, Research Triangle Park, NC 27709, United States
[b] Chemical Computing Group, Suite 910, 1010 Sherbrooke Street West, Montreal, QC H3A 2R7, Canada
[c] Oak Ridge Institute for Science and Education, 109 T.W. Alexander Drive, Research Triangle Park, NC 27709, United States
[d] Student Services Contractor, U.S. Environmental Protection Agency, 109 T.W. Alexander Drive, Research Triangle Park, NC 27709, United States
[e] ICF International, 2635 Meridian Pkwy #200, Durham, NC 27713, United States
[f] U.S. Environmental Protection Agency, Office of Research and Development, National Center for Computational Toxicology, 109 T.W. Alexander Drive, Research Triangle Park, NC 27709, United States


Green Chemistry

PAPER

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View Journal | View Issue

Cite this: Green Chem., 2017, 19, 1063

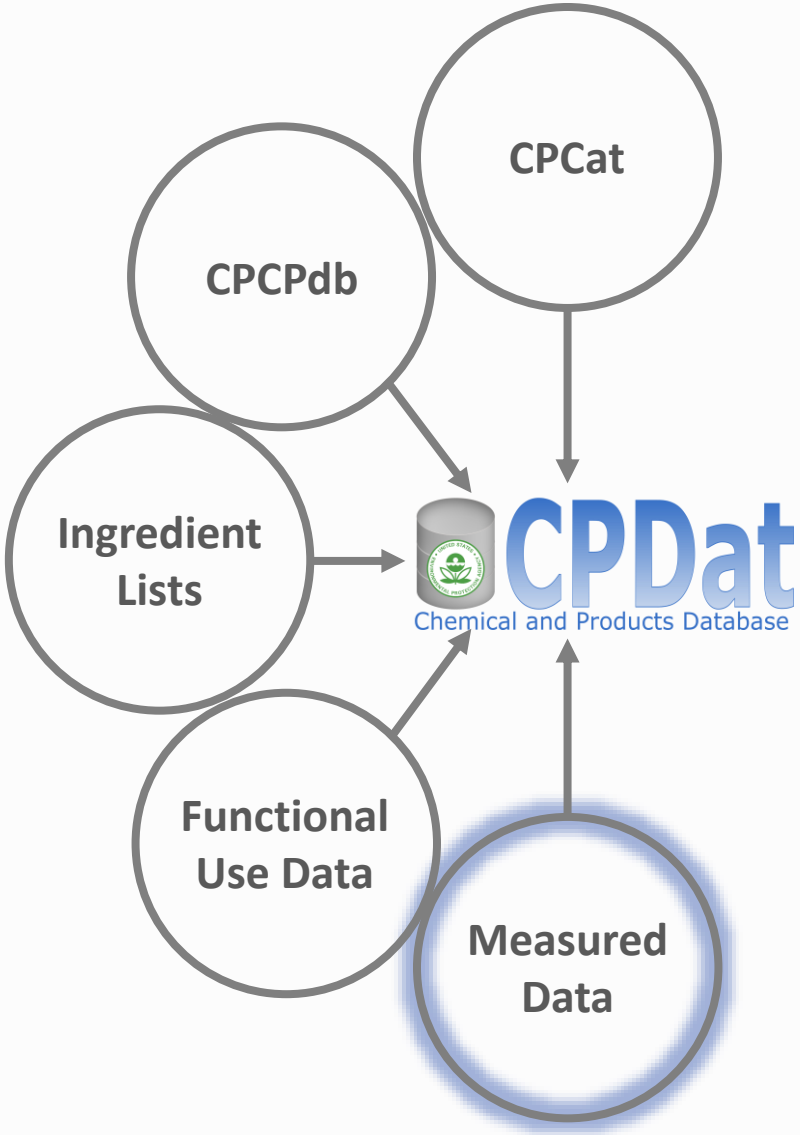
High-throughput screening of chemicals as functional substitutes using structure-based classification models†

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

Categorization by functional use

- Reported functional use
- Harmonized functional use
- Predicted functional uses based on structure

What is CPDat?



Environmental Science & Technology
Article
Cite This: Environ. Sci. Technol. 2018, 52, 3125−3135
pubs.acs.org/est

Suspect Screening Analysis of Chemicals in Consumer Products

Katherine A. Phillips,[†] Alice Yau,[‡] Kristin A. Favela,[‡] Kristin K. Isaacs,[†] Andrew McEachran,[§,∥] Christopher Grulke,[∥] Ann M. Richard,[∥] Antony J. Williams,[∥] Jon R. Sobus,[†] Russell S. Thomas,[∥] and John F. Wambaugh*[,∥]

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[‡]Southwest Research Institute, San Antonio, Texas 78238, United States

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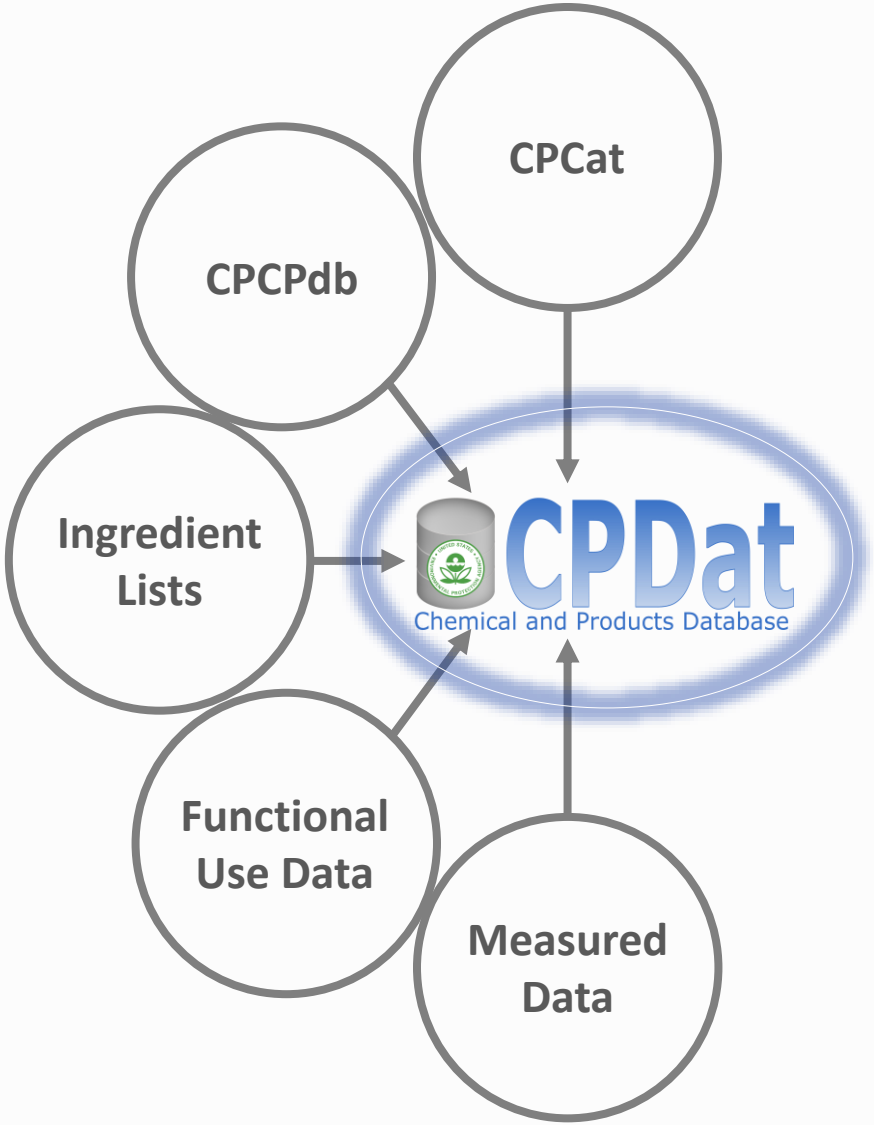
[∥]National Center for Computational Toxicology, Office of Research and Development, U.S. Environmental Protection Agency, 109 T. W. Alexander Drive, Research Triangle Park, North Carolina 27711, United States

Targeted and non-targeted measurement of chemicals in consumer products

- Measured weight fractions
- Confirmed presence
- Tentative identification

What is CPDat?



SCIENTIFIC DATA

OPEN

Received: 16 October 2017
Accepted: 30 April 2018
Published: 10 July 2018

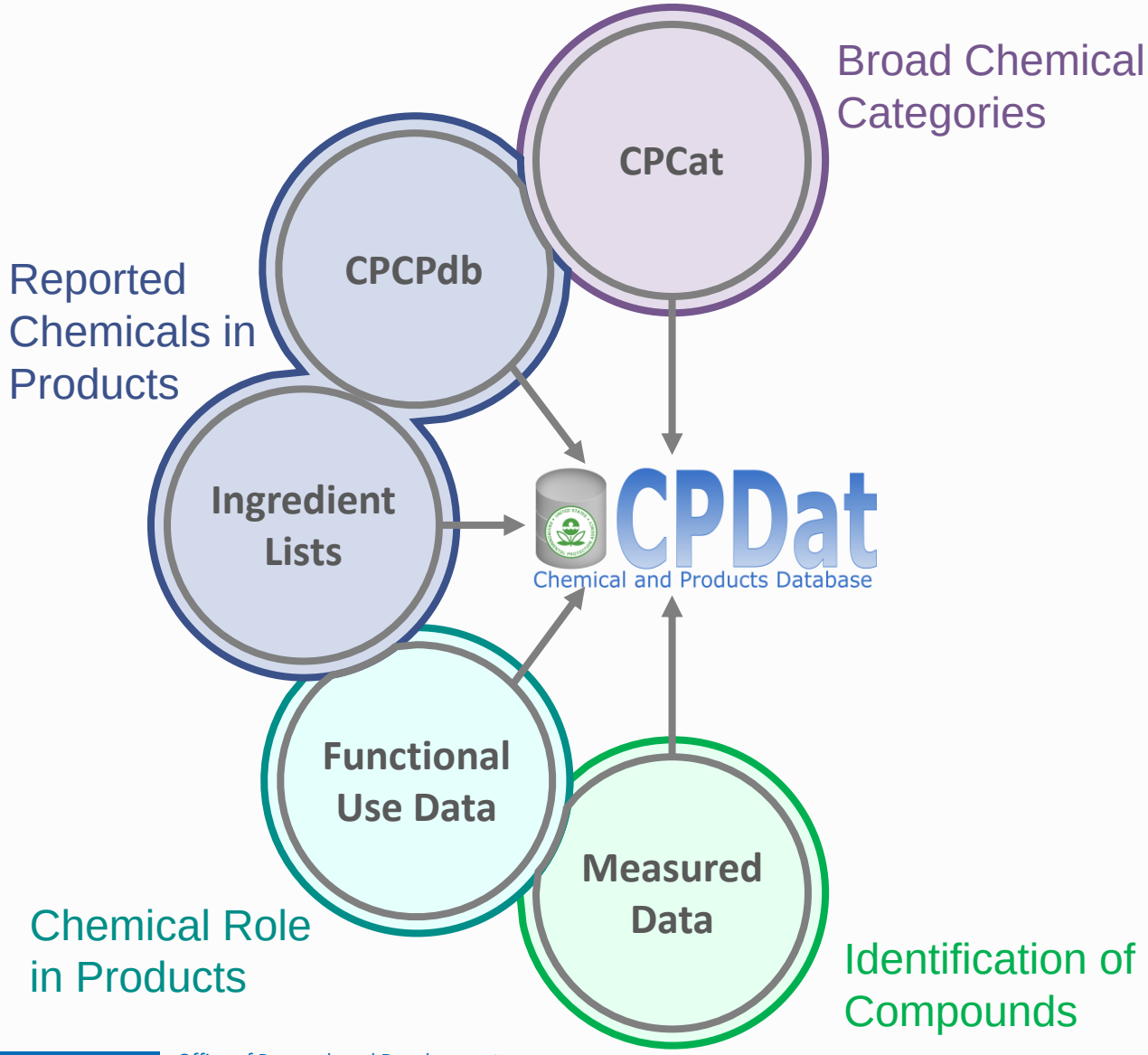
Data Descriptor: The Chemical and Products Database, a resource for exposure-relevant data on chemicals in consumer products

Kathie L. Dionisio[1], Katherine Phillips[1], Paul S. Price[1], Christopher M. Grulke[2], Antony Williams[2], Derya Biryol[1,3], Tao Hong[4] & Kristin K. Isaacs[1]

Quantitative data on product chemical composition is a necessary parameter for characterizing near-field exposure. This data set comprises reported and predicted information on more than 75,000 chemicals and more than 15,000 consumer products. The data's primary intended use is for exposure, risk, and safety assessments. The data set includes specific products with quantitative or qualitative ingredient information, which has been publicly disclosed through material safety data sheets (MSDS) and ingredient lists. A single product category from a refined and harmonized set of categories has been assigned to each product. The data set also contains information on the functional role of chemicals in products, which can inform predictions of the concentrations in which they occur. These data will be useful to exposure and risk assessors evaluating chemical and product safety.

- Broad categorization of chemical use
- Comprehensive hierarchical categorization of chemical usage by consumer product type
- Functional use of chemicals
- Quantitative chemical composition for consumer products

What is CPDat?

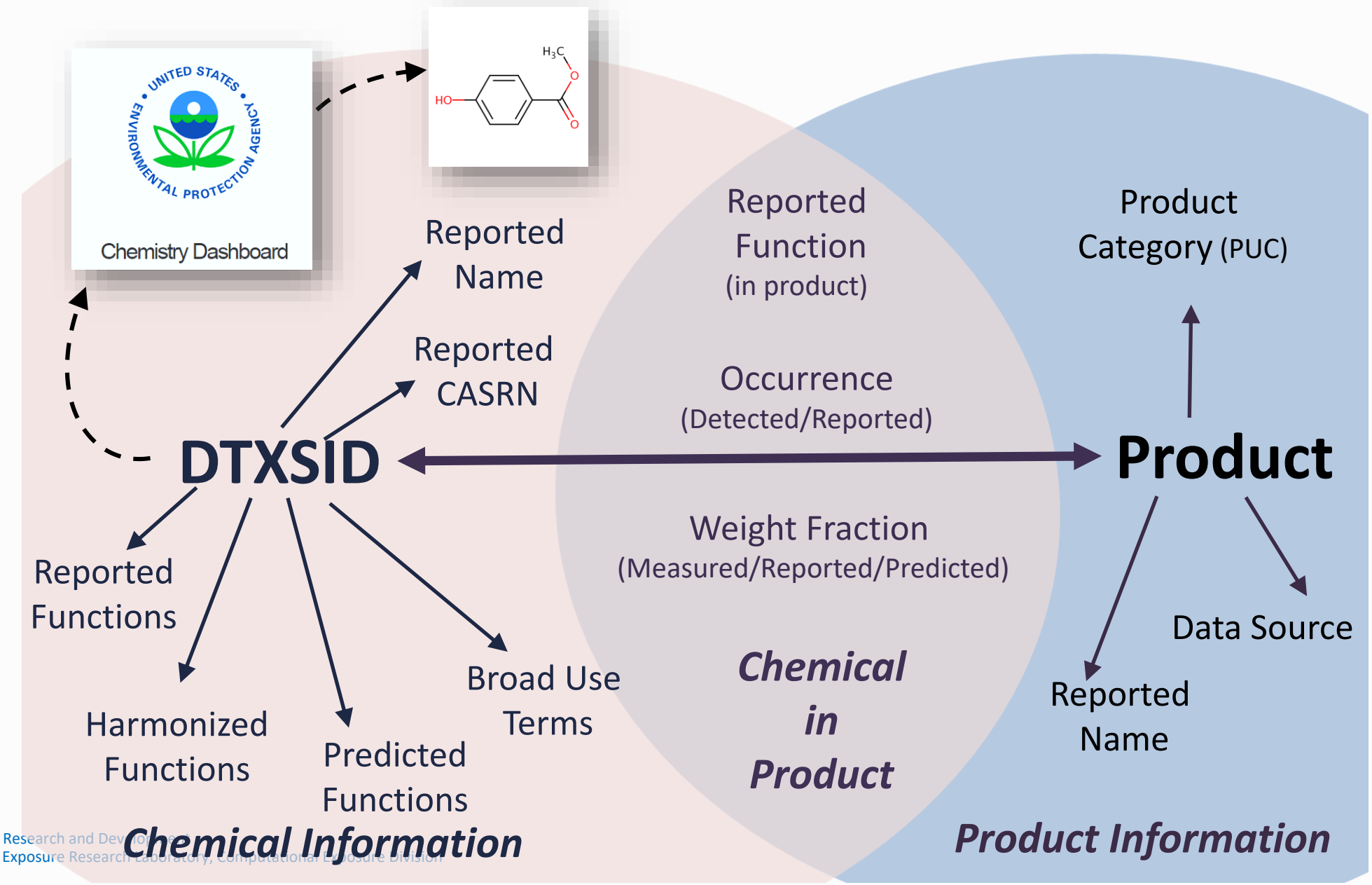


30,000-60,000 chemicals

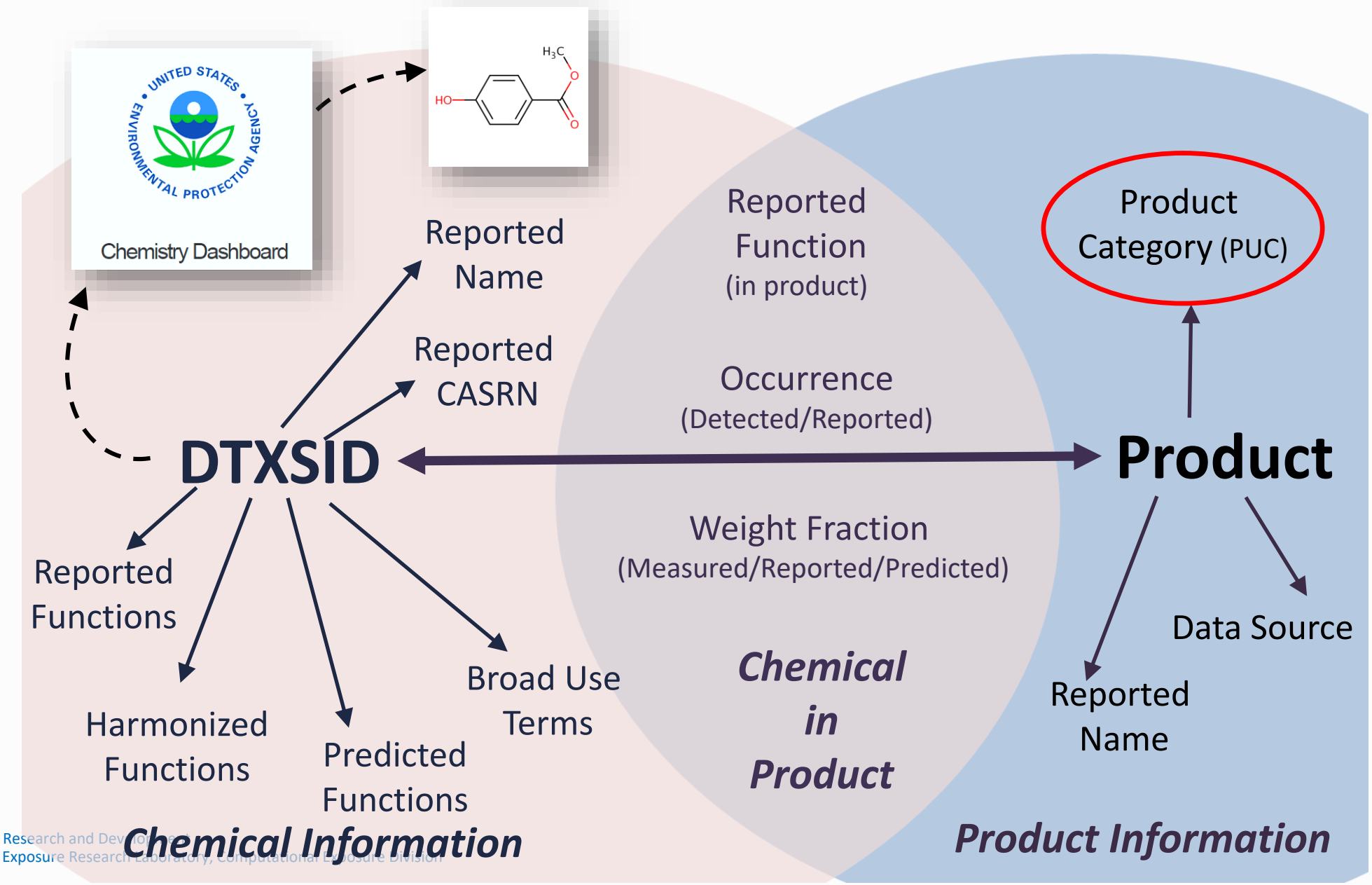
16,000 products

~200 consumer product categories

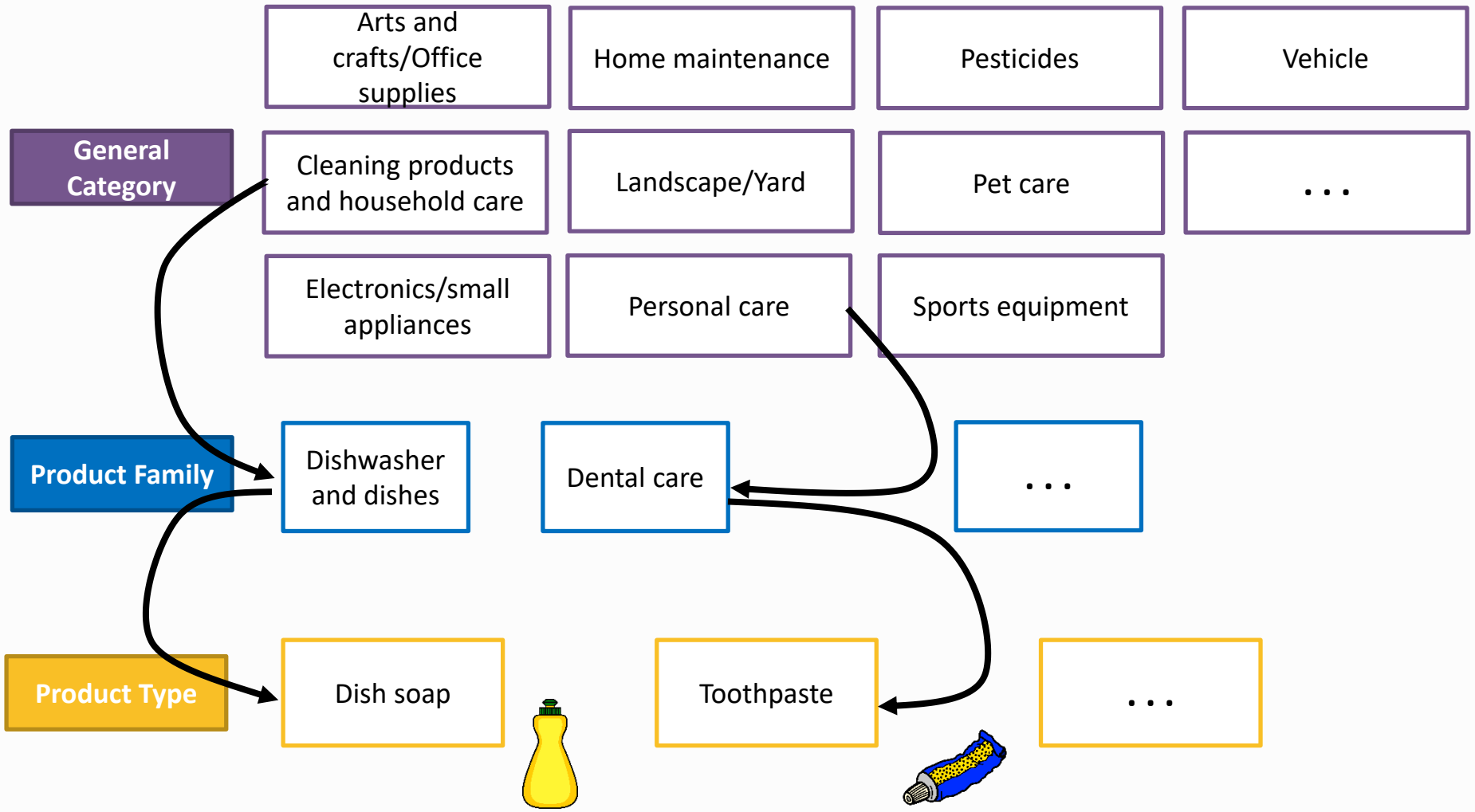
Information linkages in CPDat



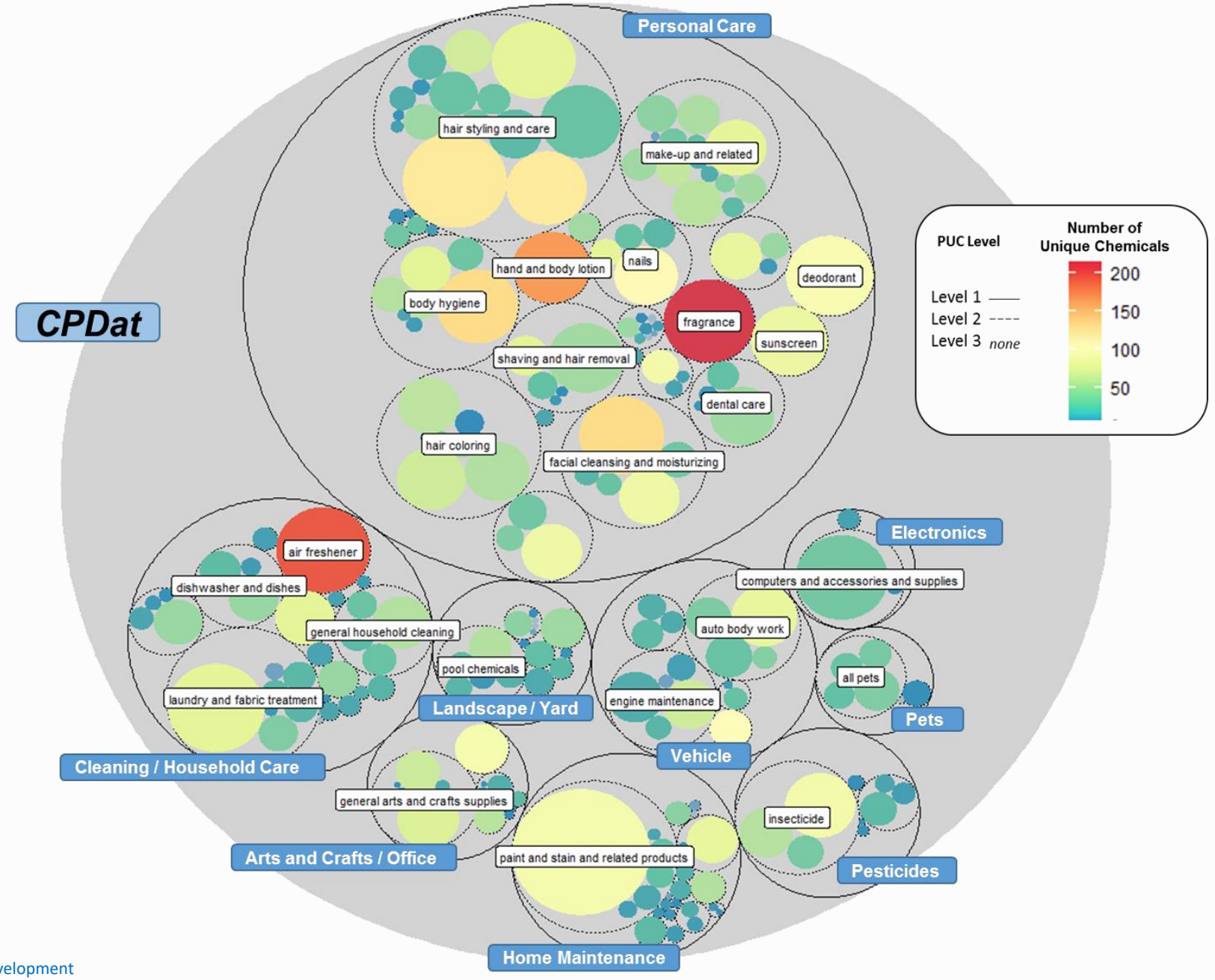
Information linkages in CPDat



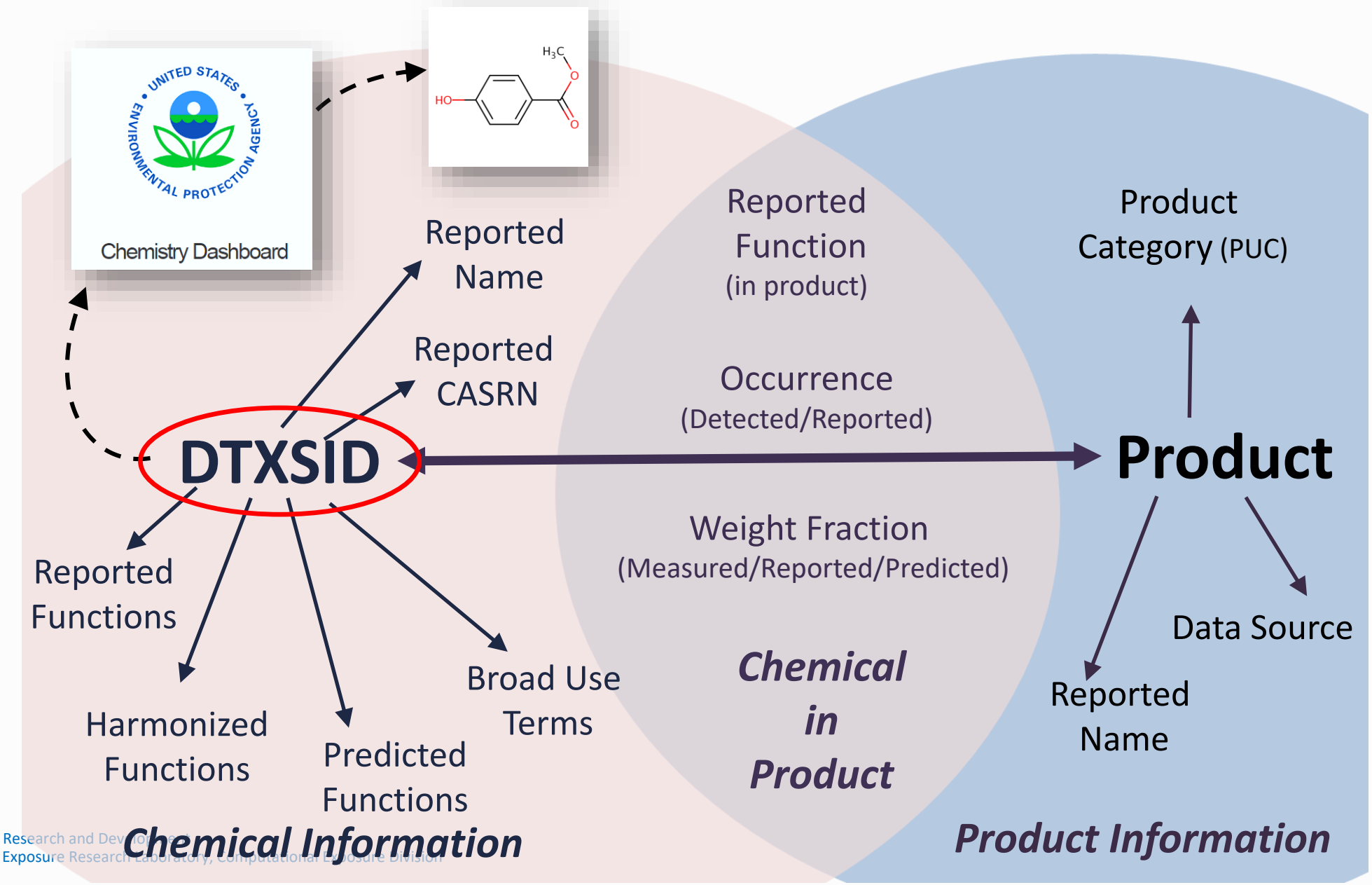
Product Use Categories (PUCs) in CPDat



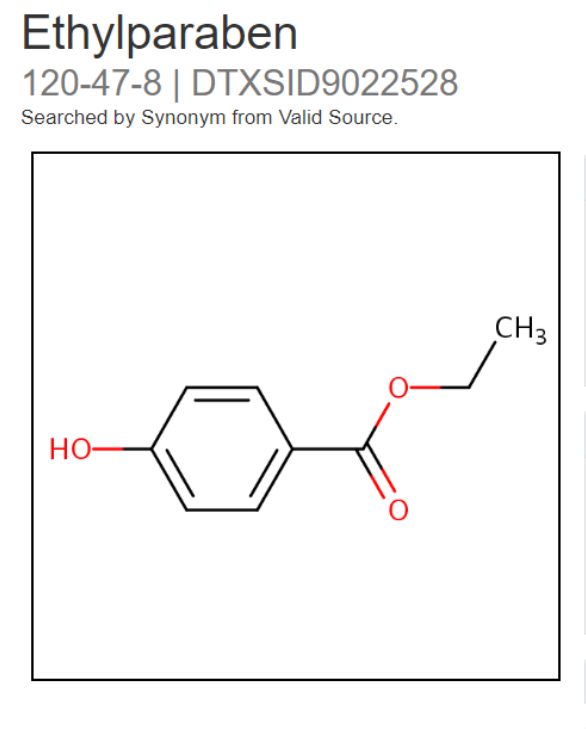
- PUCs group products based on
  - Meeting a common need
  - Having similar routes of exposures
- PUCs are consistent with harmonized OECD system of product categorizations for chemical reporting
- Hierarchy based system


CPDat
Personal Care
hair styling and care
make-up and related
hand and body lotion
nails
deodorant
body hygiene
fragrance
sunscreen
shaving and hair removal
dental care
hair coloring
facial cleansing and moisturizing
PUC Level
Level 1
Level 2
Level 3 none
Number of Unique Chemicals
200
150
100
50
Electronics
computers and accessories and supplies
auto body work
all pets
Pets
engine maintenance
Vehicle
air freshener
dishwasher and dishes
general household cleaning
pool chemicals
laundry and fabric treatment
Landscape / Yard
Cleaning / Household Care
general arts and crafts supplies
Arts and Crafts / Office
insecticide
Pesticides
paint and stain and related products
Home Maintenance

Information linkages in CPDat



Chemical identification

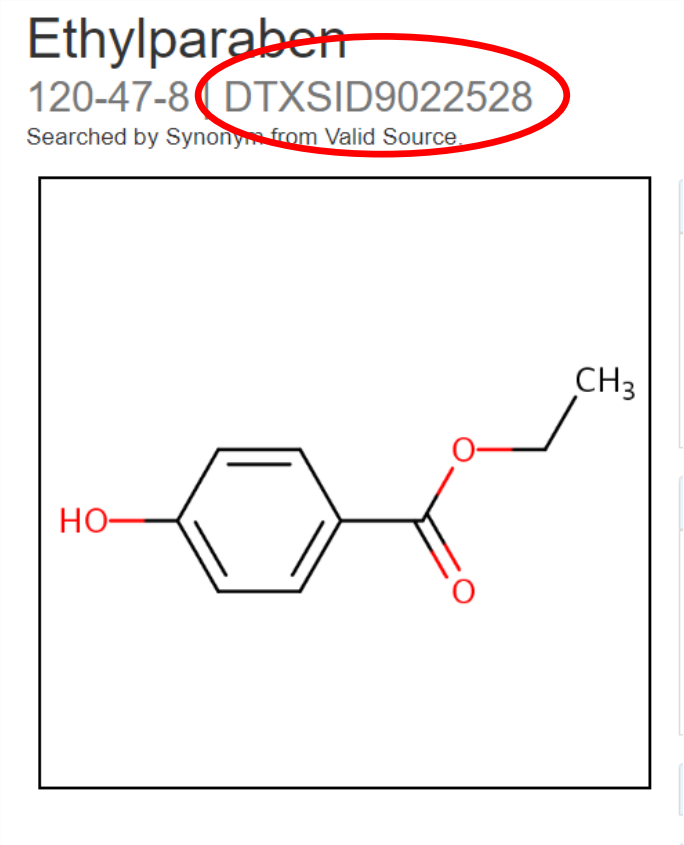


Correct chemical identification is important (and difficult!)

Potential for errors in chemical identification due to:

- Synonym chemical names
  - Ethyl 4-hydroxybenzoate
  - Benzoic acid, 4-hydroxy-, ethyl ester
  - Ethyl 4-hydroxybenzoate
- Misspelled chemical names
- Deleted and synonym CAS
- Conflicts between CAS and chemical name

Chemical identification



Correct chemical identification is important (and difficult!)

DTXSID provides unique identifier for each chemical structure

- All chemical information provided by source (CAS, chemical name) used to map substance to a DTXSID
- Conflicts are resolved

CPDat

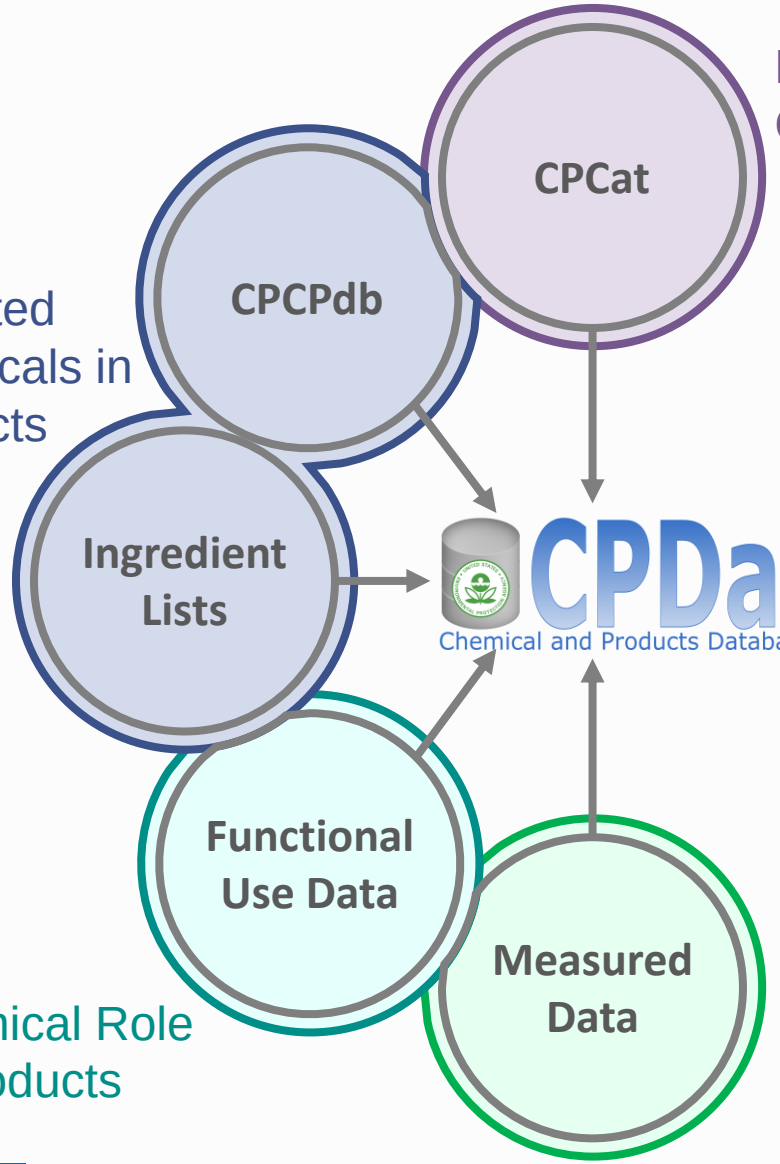
49,000 unique CAS

68,000 unique chemical names

31,000 unique substances (by DTXSID)

(+27,000 substances not yet curated)

How to access CPDat?

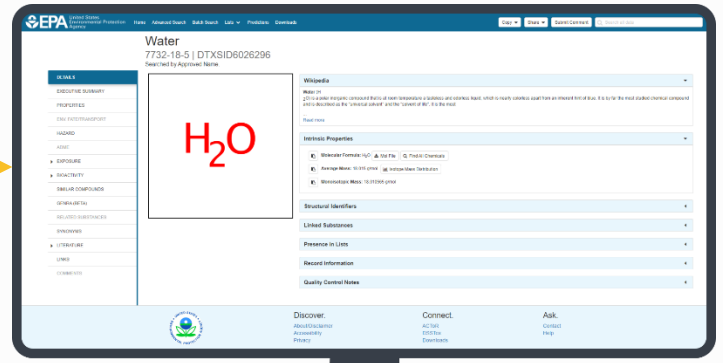


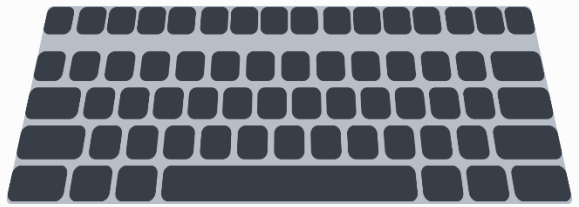
Broad Chemical Categories

Reported Chemicals in Products

Chemical Role in Products

Identification of Compounds



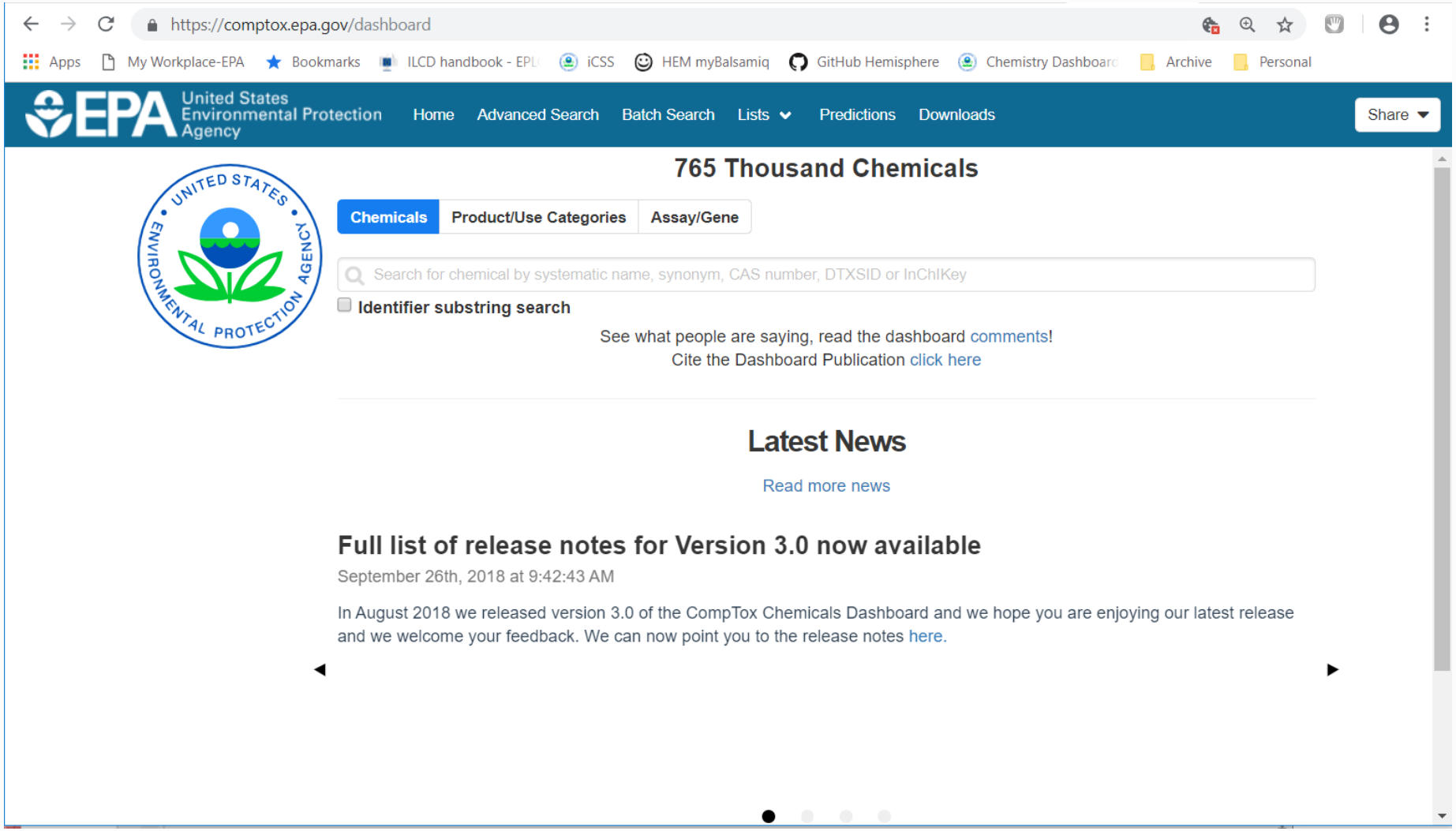


Williams et al., *J. Cheminfo.*, 2017

Freely search, explore, and use our data

https://comptox.epa.gov/dashboard

How to access CPDat?



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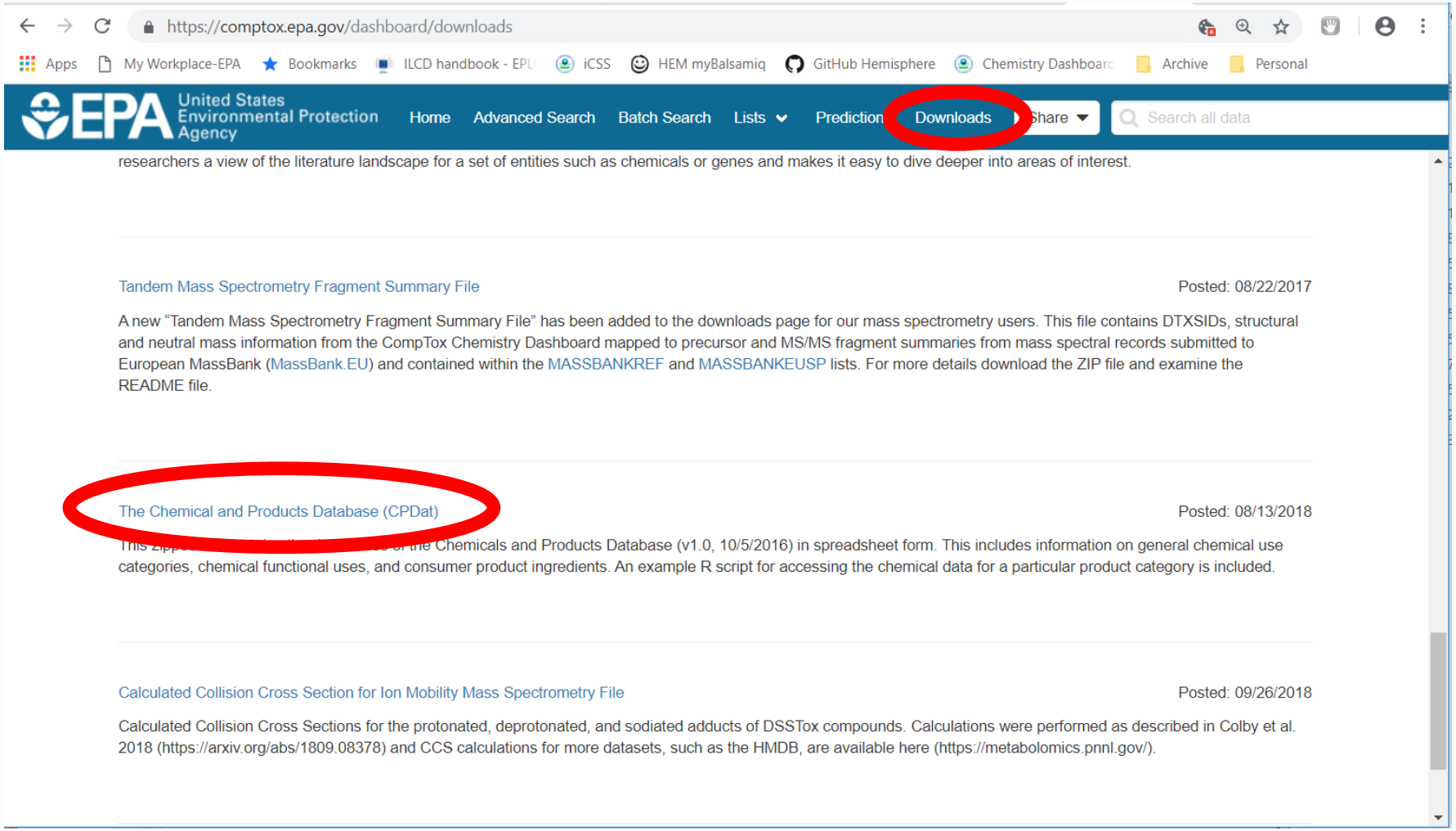
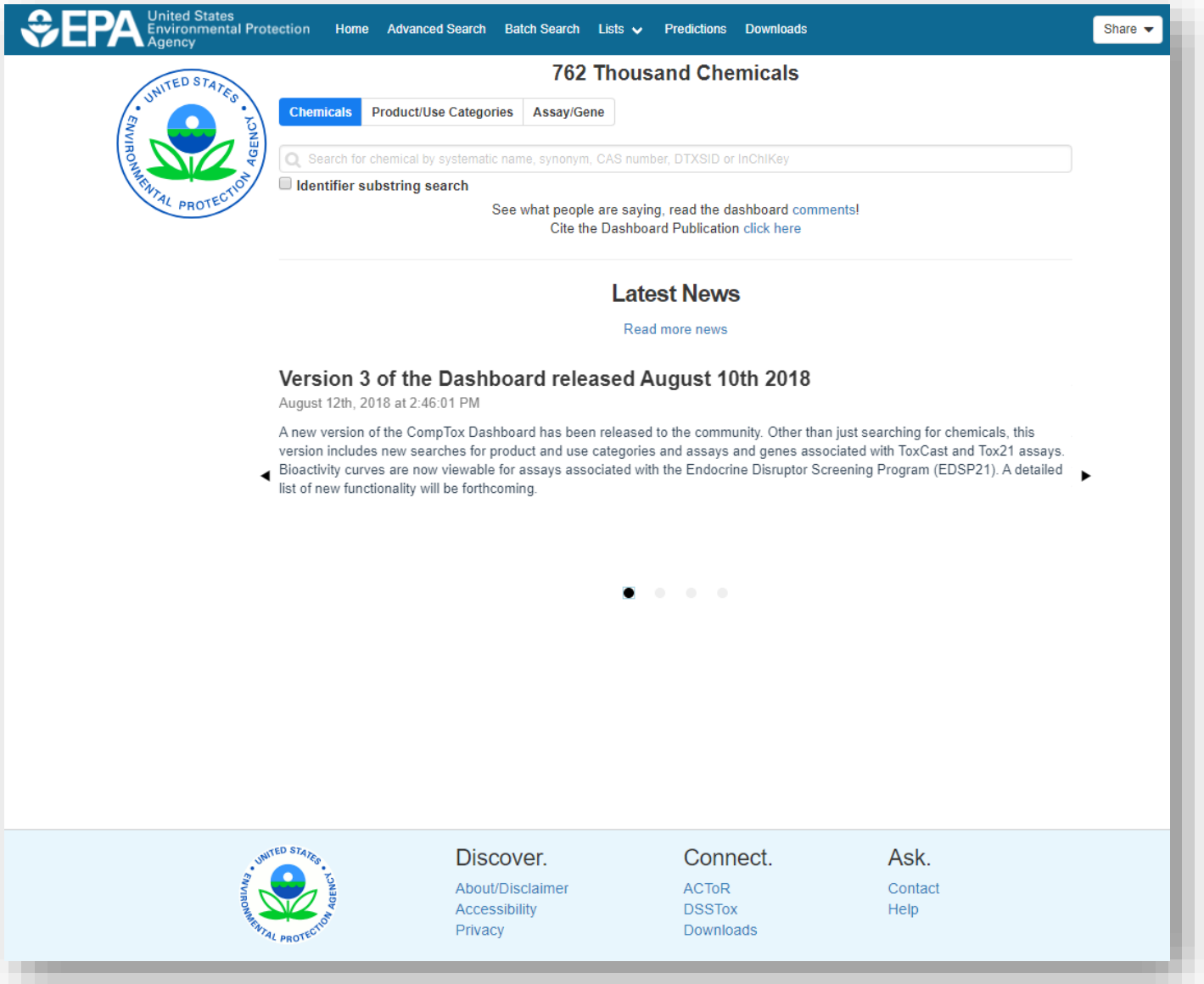
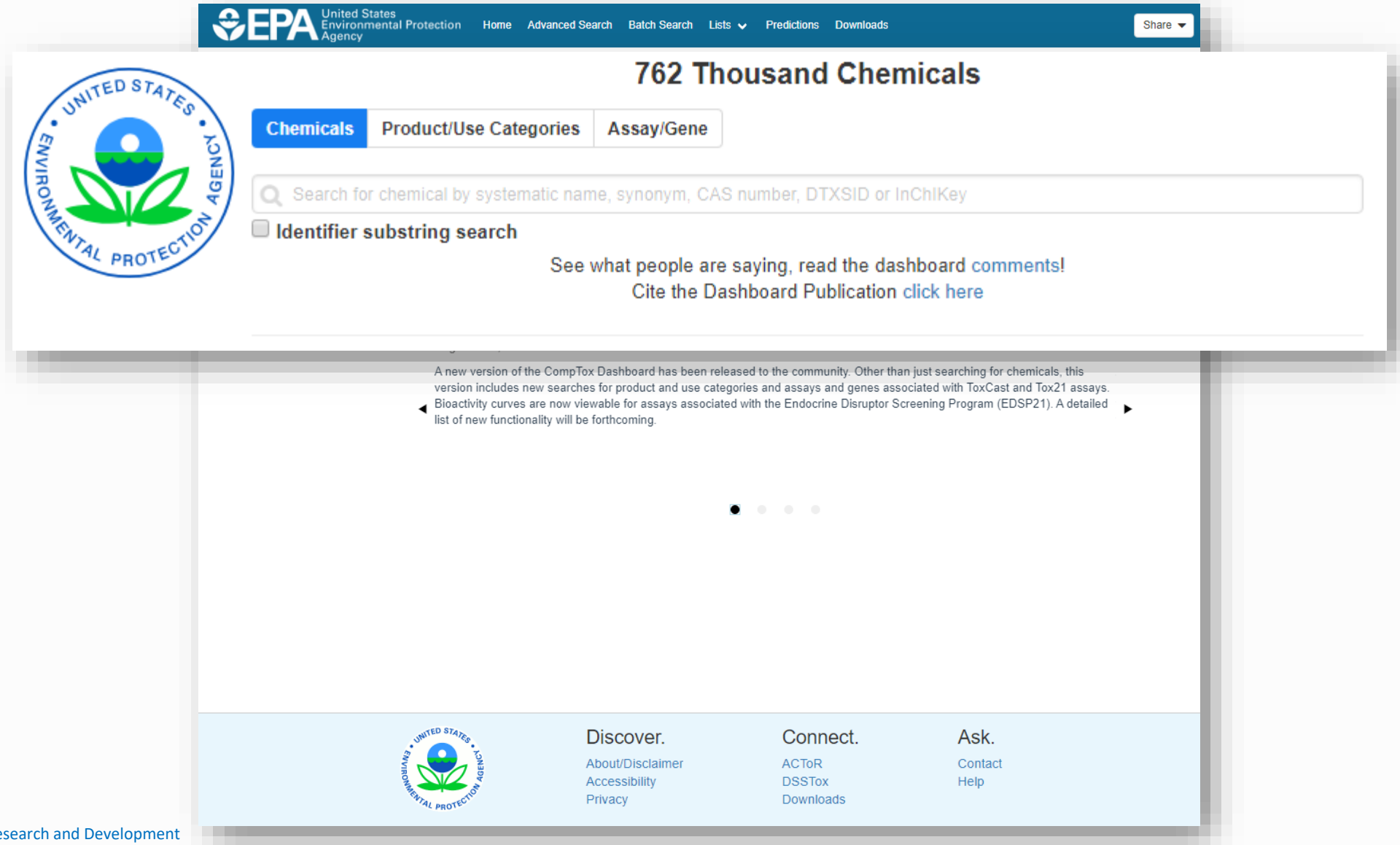


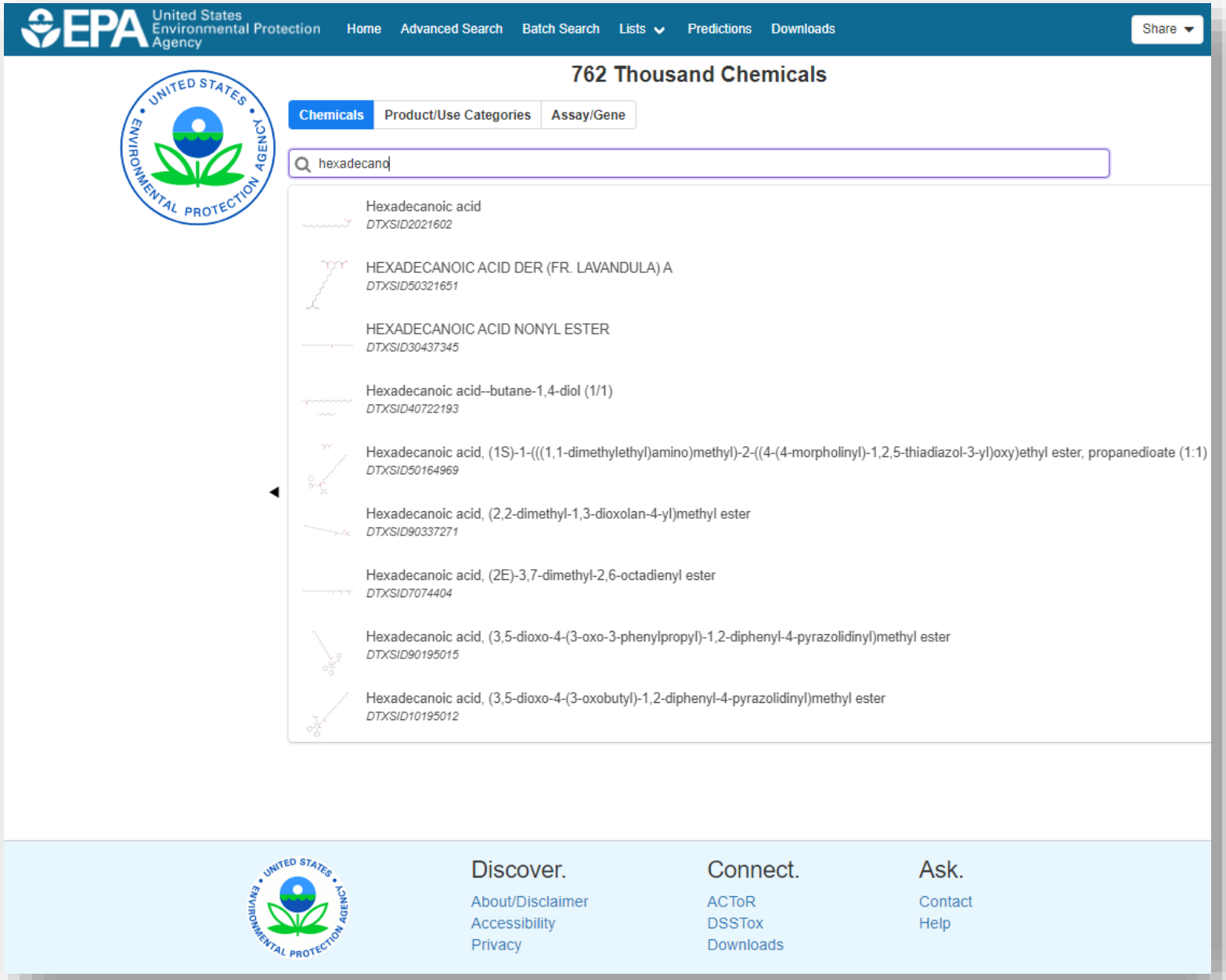
https://comptox.epa.gov/dashboard/downloads

Using the CompTox Chemicals Dashboard to access CPDat



Searching by chemical




EPA United States Environmental Protection Agency
Home
Advanced Search
Batch Search
Lists
Predictions
Downloads
Share
762 Thousand Chemicals
Chemicals
Product/Use Categories
Assay/Gene
hexadecano
Hexadecanoic acid
DTXSID2021602
HEXADECANOIC ACID DER (FR. LAVANDULA) A
DTXSID50321651
HEXADECANOIC ACID NONYL ESTER
DTXSID30437345
Hexadecanoic acid--butane-1,4-diol (1/1)
DTXSID40722193
Hexadecanoic acid, (1S)-1-(((1,1-dimethylethyl)amino)methyl)-2-((4-(4-morpholinyl)-1,2,5-thiadiazol-3-yl)oxy)ethyl ester, propanedioate (1:1)
DTXSID50164969
Hexadecanoic acid, (2,2-dimethyl-1,3-dioxolan-4-yl)methyl ester
DTXSID90337271
Hexadecanoic acid, (2E)-3,7-dimethyl-2,6-octadienyl ester
DTXSID7074404
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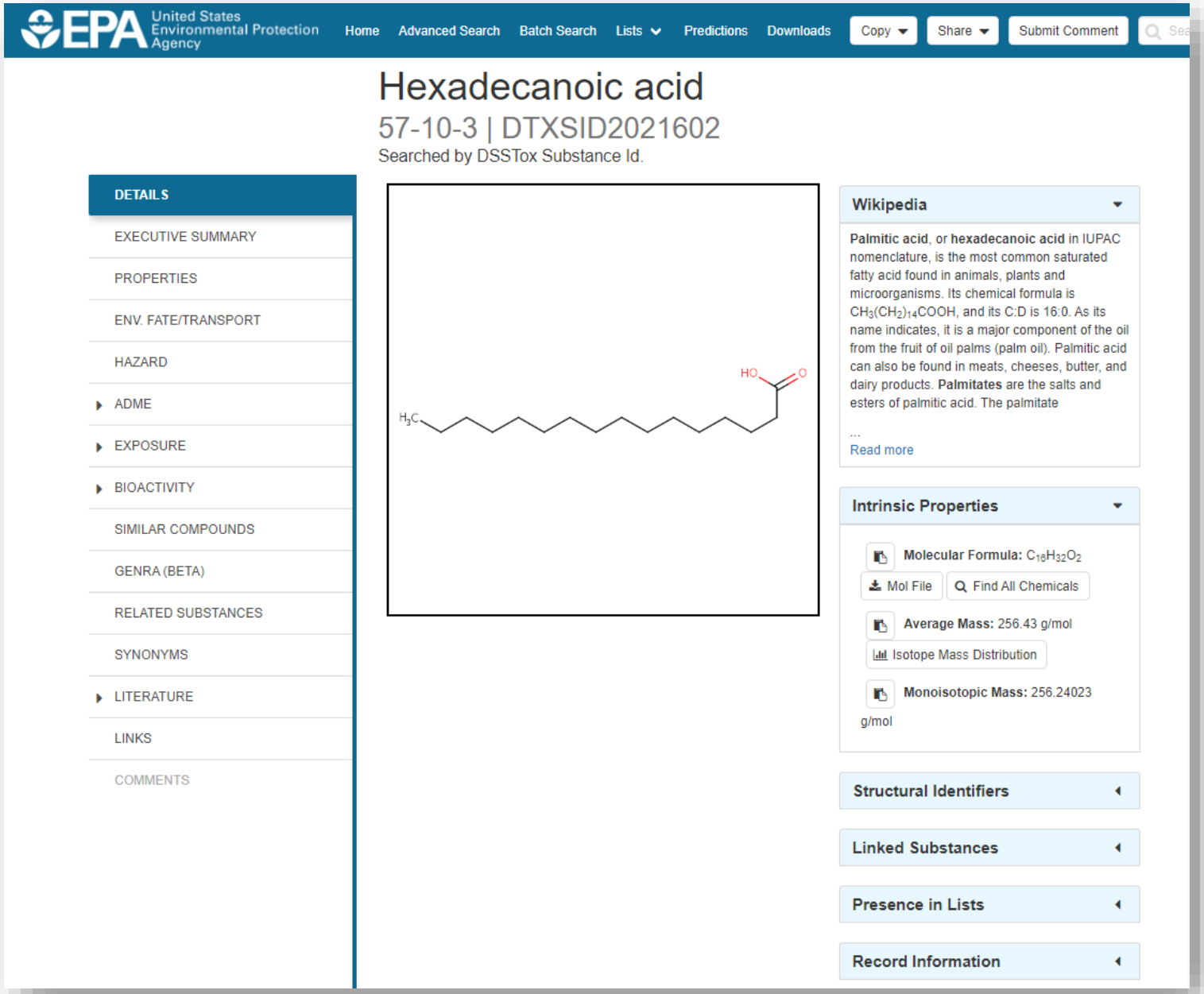
DTXSID90195015
Hexadecanoic acid, (3,5-dioxo-4-(3-oxobutyl)-1,2-diphenyl-4-pyrazolidinyl)methyl ester
DTXSID10195012
Discover.
About/Disclaimer
Accessibility
Privacy
Connect.
ACToR
DSSTox
Downloads
Ask.
Contact
Help


EPA United States Environmental Protection Agency
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Advanced Search
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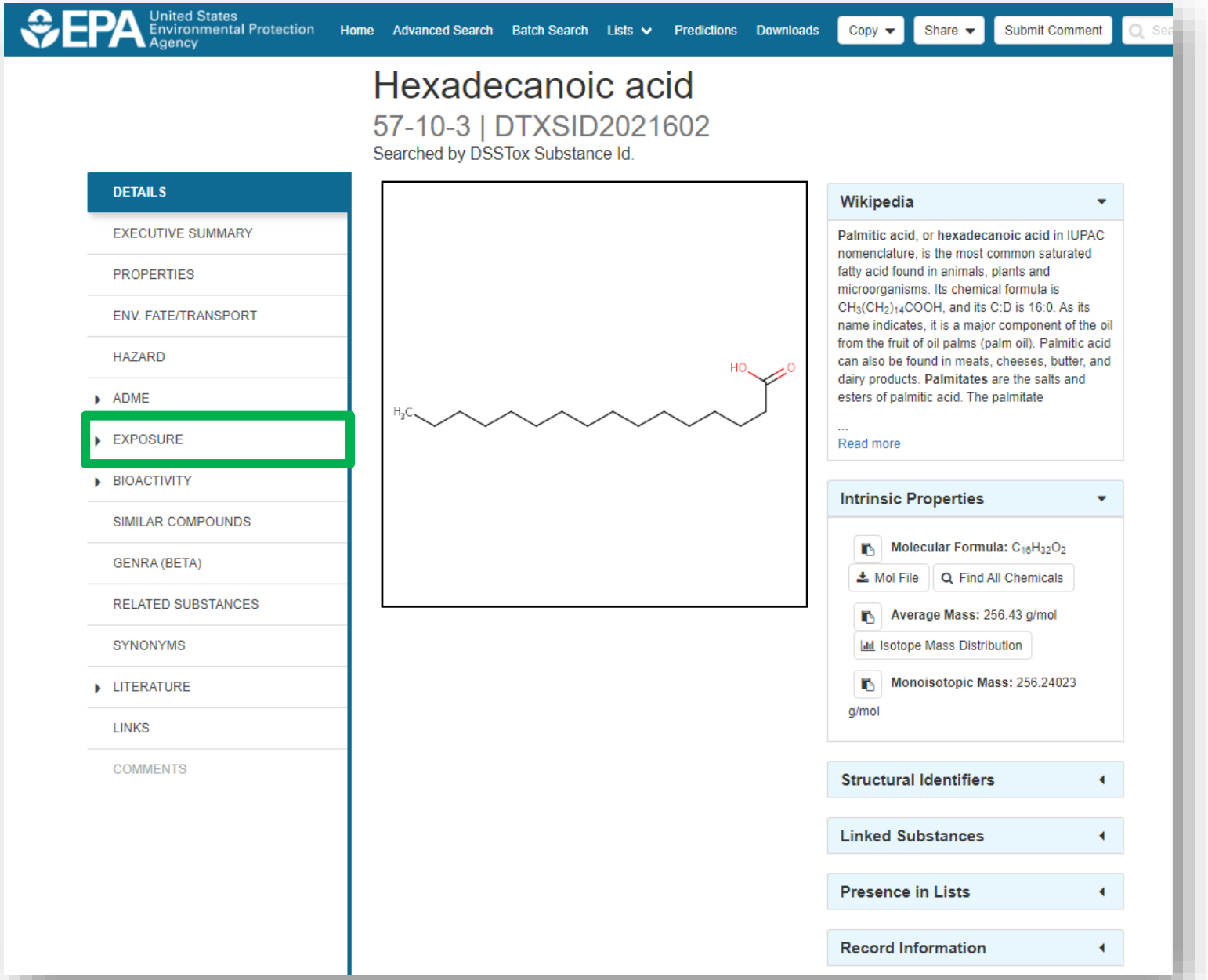
Lists
Predictions
Downloads
Copy
Share
Submit Comment
Hexadecanoic acid
57-10-3 | DTXSID2021602
Searched by DSSTox Substance Id.
DETAILS
EXECUTIVE SUMMARY
PROPERTIES
ENV. FATE/TRANSPORT
HAZARD
ADME
EXPOSURE
BIOACTIVITY
SIMILAR COMPOUNDS
GENRA (BETA)
RELATED SUBSTANCES
SYNONYMS
LITERATURE
LINKS
COMMENTS
HO
O
H3C
Wikipedia
Palmitic acid, or hexadecanoic acid in IUPAC nomenclature, is the most common saturated fatty acid found in animals, plants and microorganisms. Its chemical formula is CH3(CH2)14COOH, and its C:D is 16:0. As its name indicates, it is a major component of the oil from the fruit of oil palms (palm oil). Palmitic acid can also be found in meats, cheeses, butter, and dairy products. Palmitates are the salts and esters of palmitic acid. The palmitate
...
Read more
Intrinsic Properties
Molecular Formula: C16H32O2
Mol File
Find All Chemicals
Average Mass: 256.43 g/mol
Isotope Mass Distribution
Monoisotopic Mass: 256.24023 g/mol
Structural Identifiers
Linked Substances
Presence in Lists
Record Information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57-10-3 | DTXSID2021602
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HAZARD
ADME
EXPOSURE
BIOACTIVITY
SIMILAR COMPOUNDS
GENRA (BETA)
RELATED SUBSTANCES
SYNONYMS
LITERATURE
LINKS
COMMENTS
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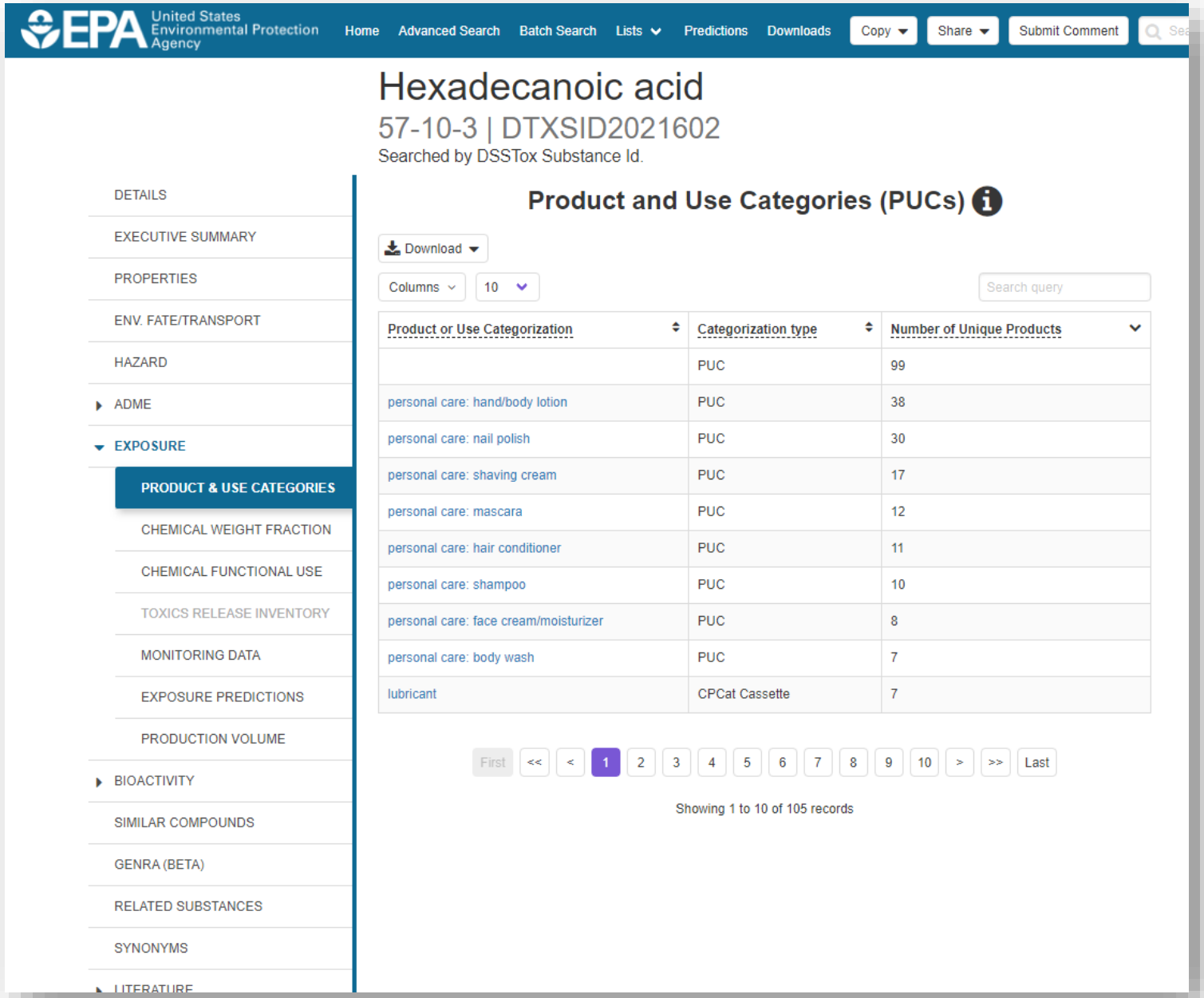
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PRODUCT & USE CATEGORIES
CHEMICAL WEIGHT FRACTION
CHEMICAL FUNCTIONAL USE
TOXICS RELEASE INVENTORY
MONITORING DATA
EXPOSURE PREDICTIONS
PRODUCTION VOLUME
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SIMILAR COMPOUNDS
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RELATED SUBSTANCES
SYNONYMS
LITERATURE
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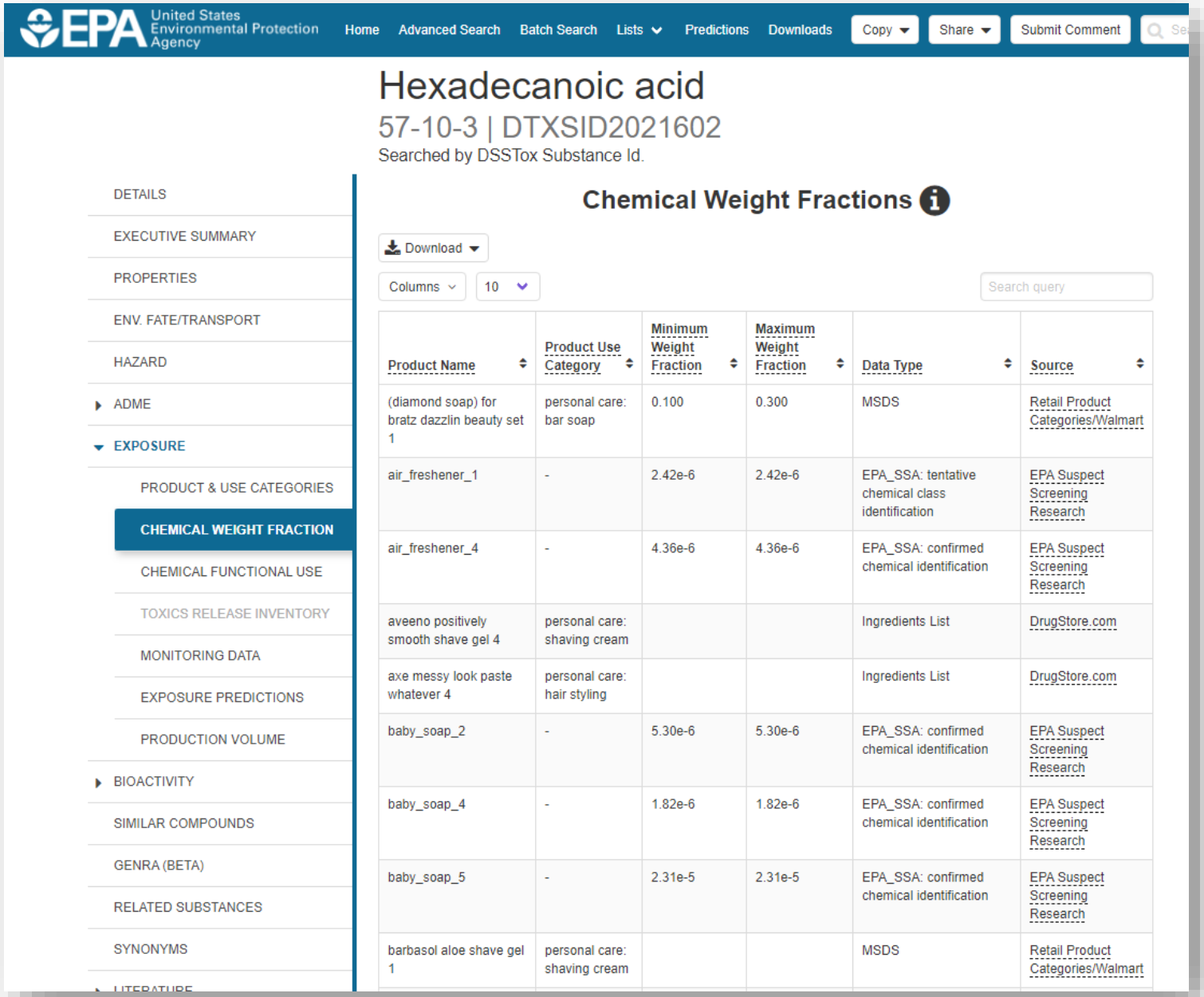
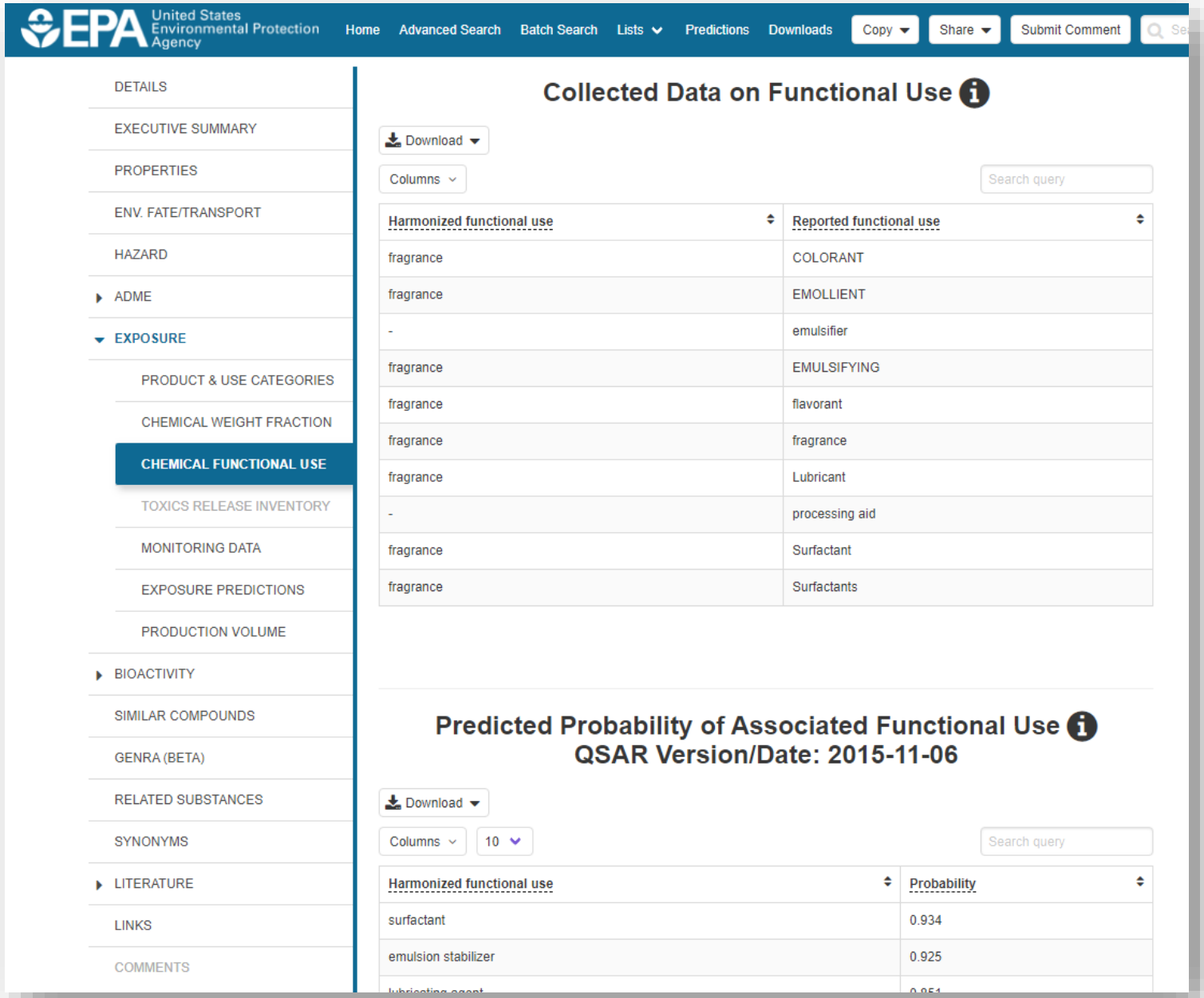
10
Search query
Product or Use Categorization
Categorization type
Number of Unique Products
PUC 99
personal care: hand/body lotion PUC 38
personal care: nail polish PUC 30
personal care: shaving cream PUC 17
personal care: mascara PUC 12
personal care: hair conditioner PUC 11
personal care: shampoo PUC 10
personal care: face cream/moisturizer PUC 8
personal care: body wash PUC 7
lubricant CPCat Cassette 7
First << < 1 2 3 4 5 6 7 8 9 10 > >> Last
Showing 1 to 10 of 105 records



Product Name	Product Use Category	Minimum Weight Fraction	Maximum Weight Fraction	Data Type	Source
(diamond soap) for bratz dazzlin beauty set 1	personal care: bar soap	0.100	0.300	MSDS	Retail Product Categories/Walmart
air_freshener_1	-	2.42e-6	2.42e-6	EPA_SSA: tentative chemical class identification	EPA Suspect Screening Research
air_freshener_4	-	4.36e-6	4.36e-6	EPA_SSA: confirmed chemical identification	EPA Suspect Screening Research
aveeno positively smooth shave gel 4	personal care: shaving cream			Ingredients List	DrugStore.com
axe messy look paste whatever 4	personal care: hair styling			Ingredients List	DrugStore.com
baby_soap_2	-	5.30e-6	5.30e-6	EPA_SSA: confirmed chemical identification	EPA Suspect Screening Research
baby_soap_4	-	1.82e-6	1.82e-6	EPA_SSA: confirmed chemical identification	EPA Suspect Screening Research
baby_soap_5	-	2.31e-5	2.31e-5	EPA_SSA: confirmed chemical identification	EPA Suspect Screening Research
barbasol aloe shave gel 1	personal care: shaving cream			MSDS	Retail Product Categories/Walmart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Reported functional use
fragrance
COLORANT
fragrance
EMOLLIENT
-
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fragrance
EMULSIFYING
fragrance
flavorant
fragrance
fragrance
fragrance
Lubricant
-
processing aid
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fragrance
Surfactants
Predicted Probability of Associated Functional Use
QSAR Version/Date: 2015-11-06
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Columns
10
Search query
Harmonized functional use
Probability
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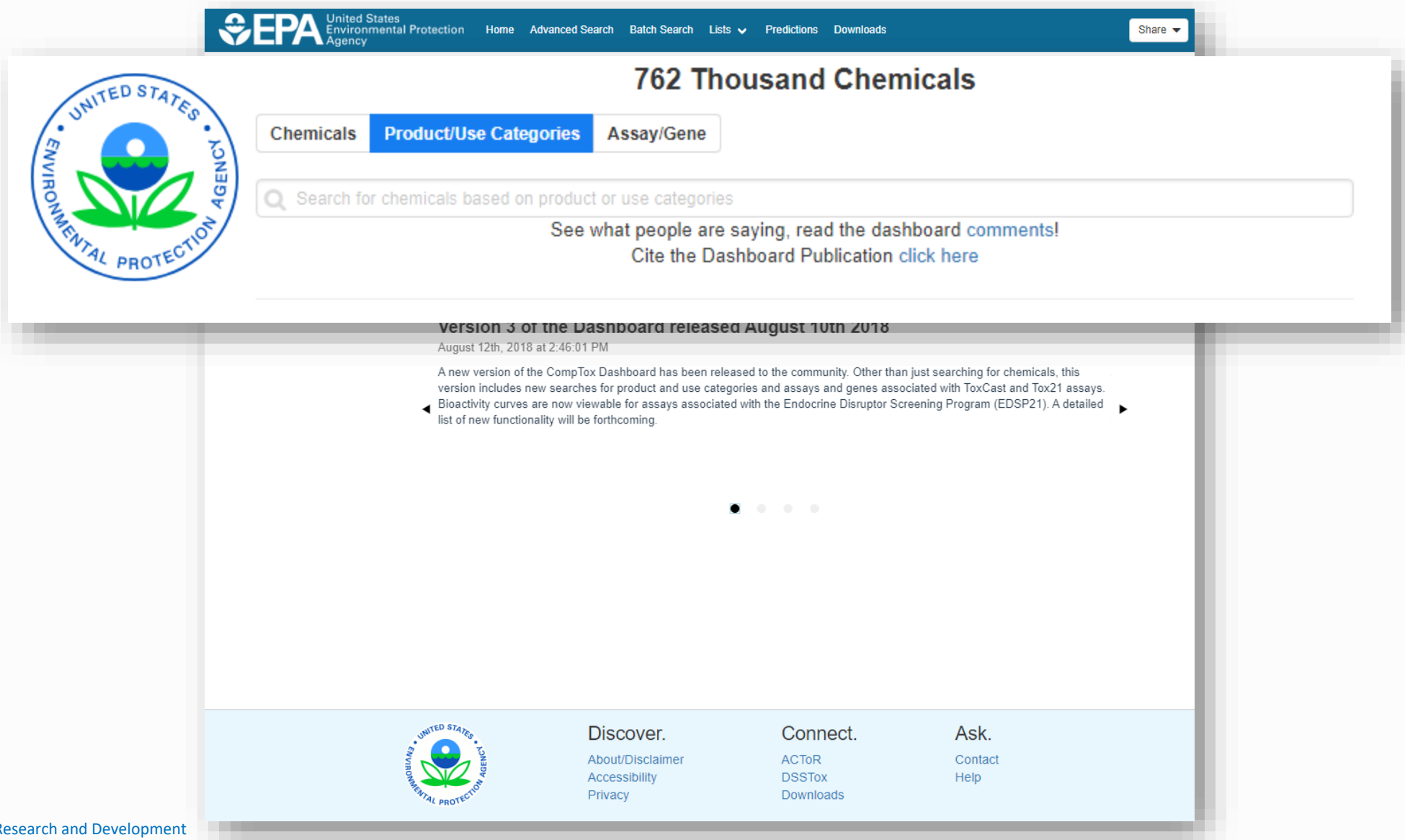
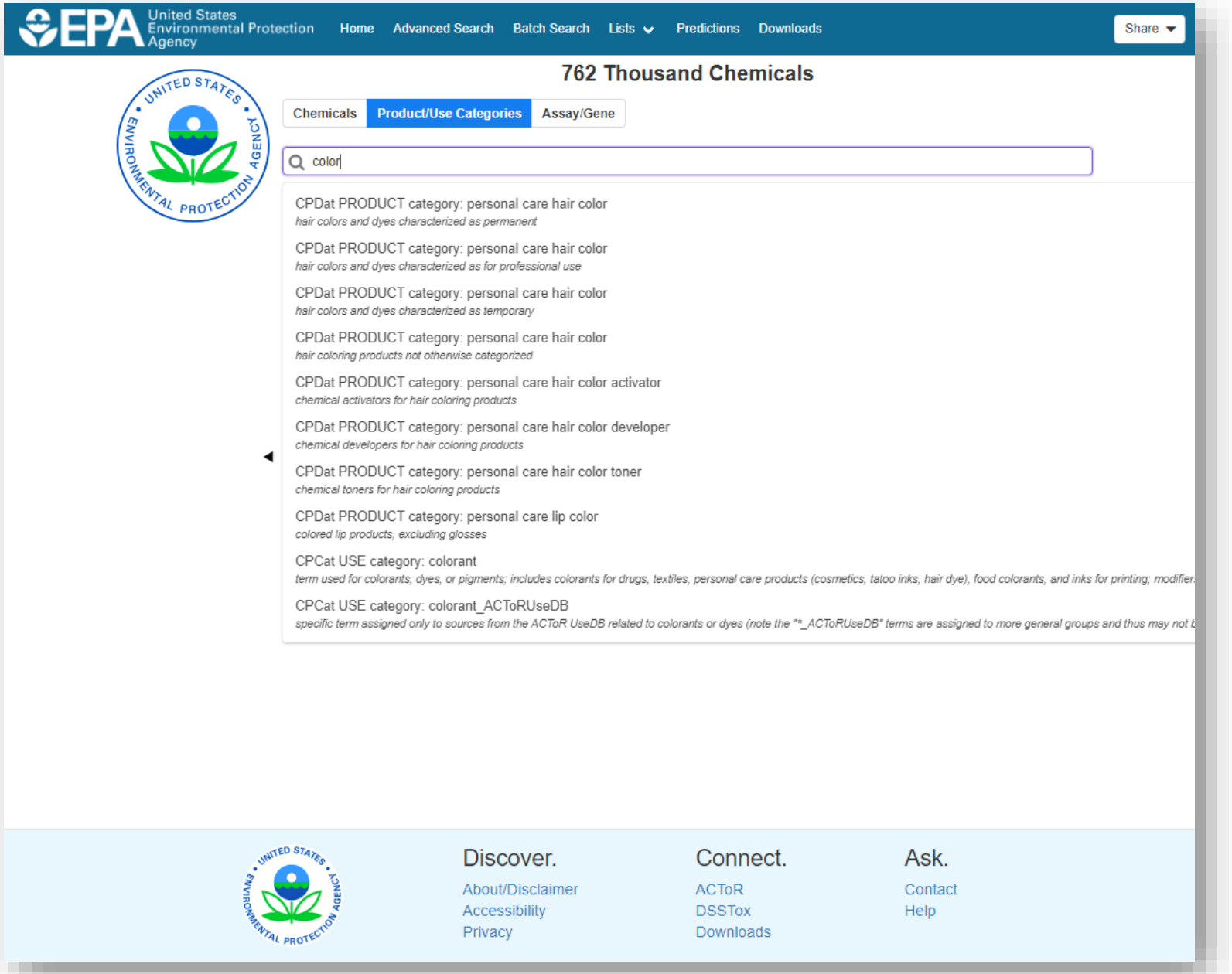
emulsion stabilizer
0.925

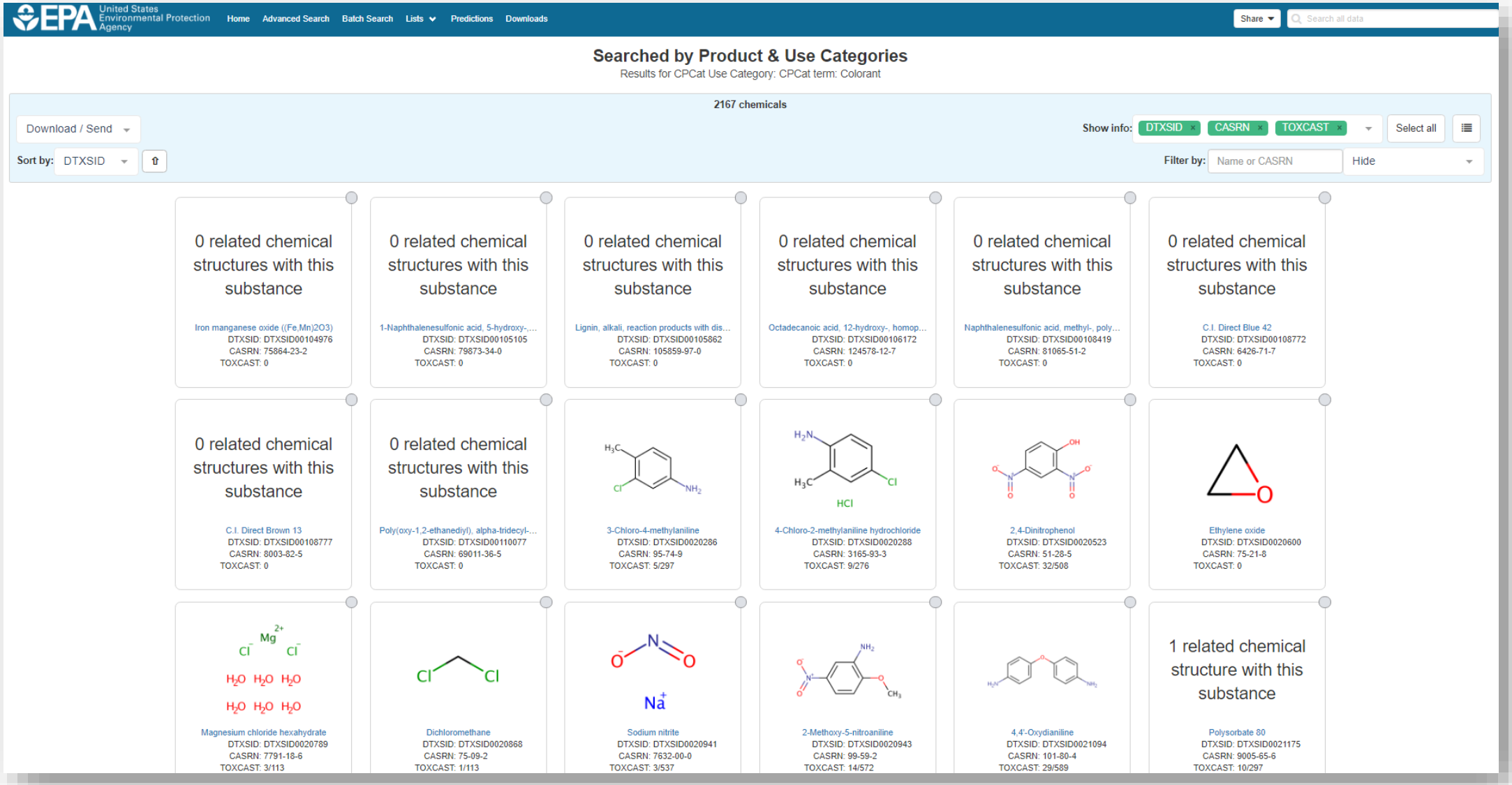
Searching by product and use categories



CPCat USE category → broad categorization of chemical use

CPDat PRODUCT category → consumer product use category (PUC)

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Searched by Product & Use Categories
Results for CPCat Use Category: CPCat term: Colorant
2167 chemicals
Download / Send
Show info:
DTXSID
CASRN
TOXCAST
Select all
Sort by:
DTXSID
Filter by:
Name or CASRN
Hide
0 related chemical structures with this substance
Iron manganese oxide ((Fe,Mn)2O3)
DTXSID: DTXSID00104976
CASRN: 75864-23-2
TOXCAST: 0
0 related chemical structures with this substance
1-Naphthalenesulfonic acid, 5-hydroxy-,...
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CASRN: 79873-34-0
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Lignin, alkali, reaction products with dis...
DTXSID: DTXSID00105862
CASRN: 105859-97-0
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Octadecanoic acid, 12-hydroxy-, homop...
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C.I. Direct Brown 13
DTXSID: DTXSID00108777
CASRN: 8003-82-5
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CASRN: 69011-36-5
TOXCAST: 0
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CASRN: 95-74-9
TOXCAST: 5/297
4-Chloro-2-methylaniline hydrochloride
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CASRN: 3165-93-3
TOXCAST: 9/276
2,4-Dinitrophenol
DTXSID: DTXSID0020523
CASRN: 51-28-5
TOXCAST: 32/508
Ethylene oxide
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TOXCAST: 0
Magnesium chloride hexahydrate
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CASRN: 7791-18-6
TOXCAST: 3/113
Dichloromethane
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CASRN: 75-09-2
TOXCAST: 1/113
Sodium nitrite
DTXSID: DTXSID0020941
CASRN: 7632-00-0
TOXCAST: 3/537
2-Methoxy-5-nitroaniline
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CASRN: 99-59-2
TOXCAST: 14/572
4,4'-Oxydianiline
DTXSID: DTXSID0021094
CASRN: 101-80-4
TOXCAST: 29/589
1 related chemical structure with this substance
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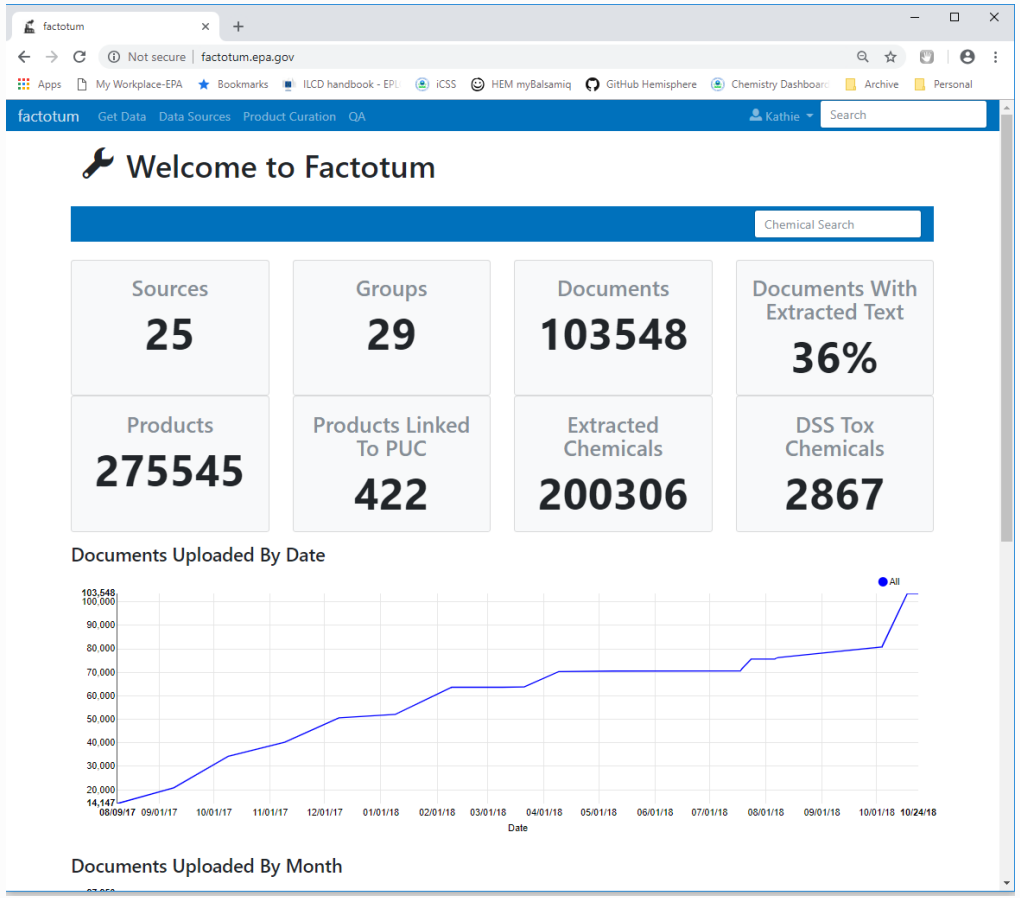
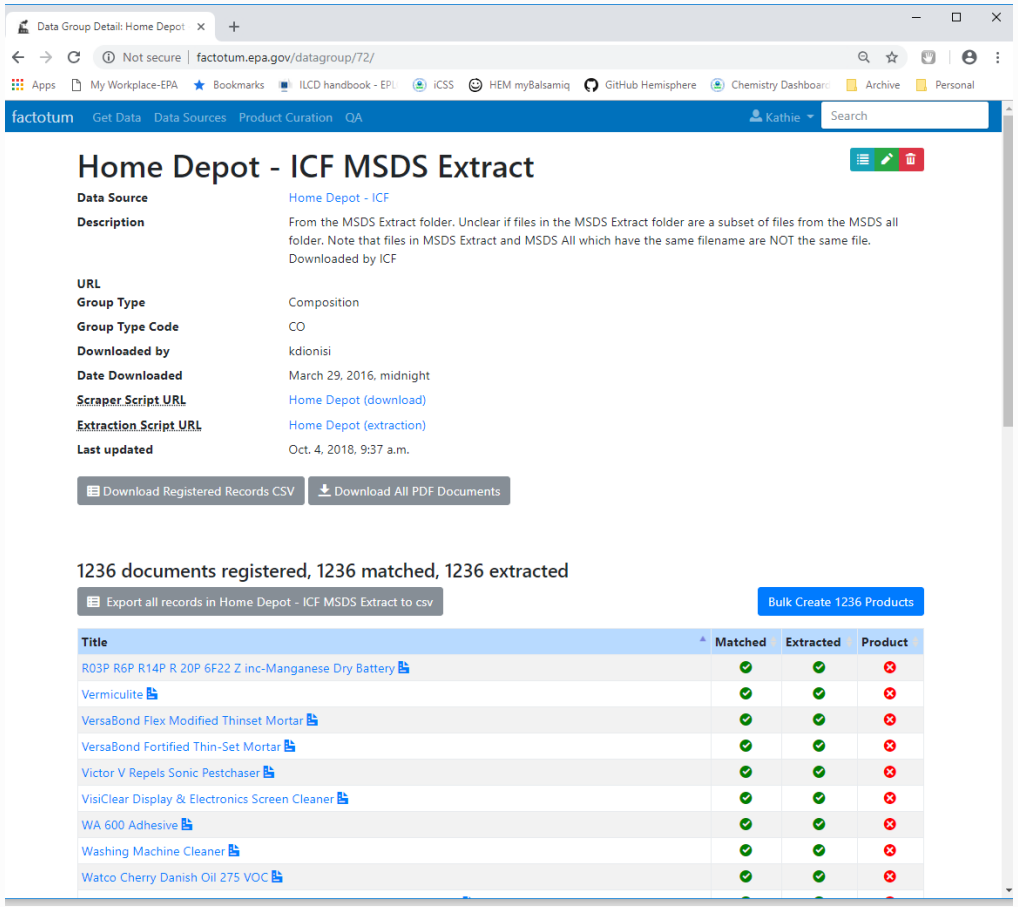
DTXSID: DTXSID0021175
CASRN: 9005-65-6
TOXCAST: 10/297

Internal data management





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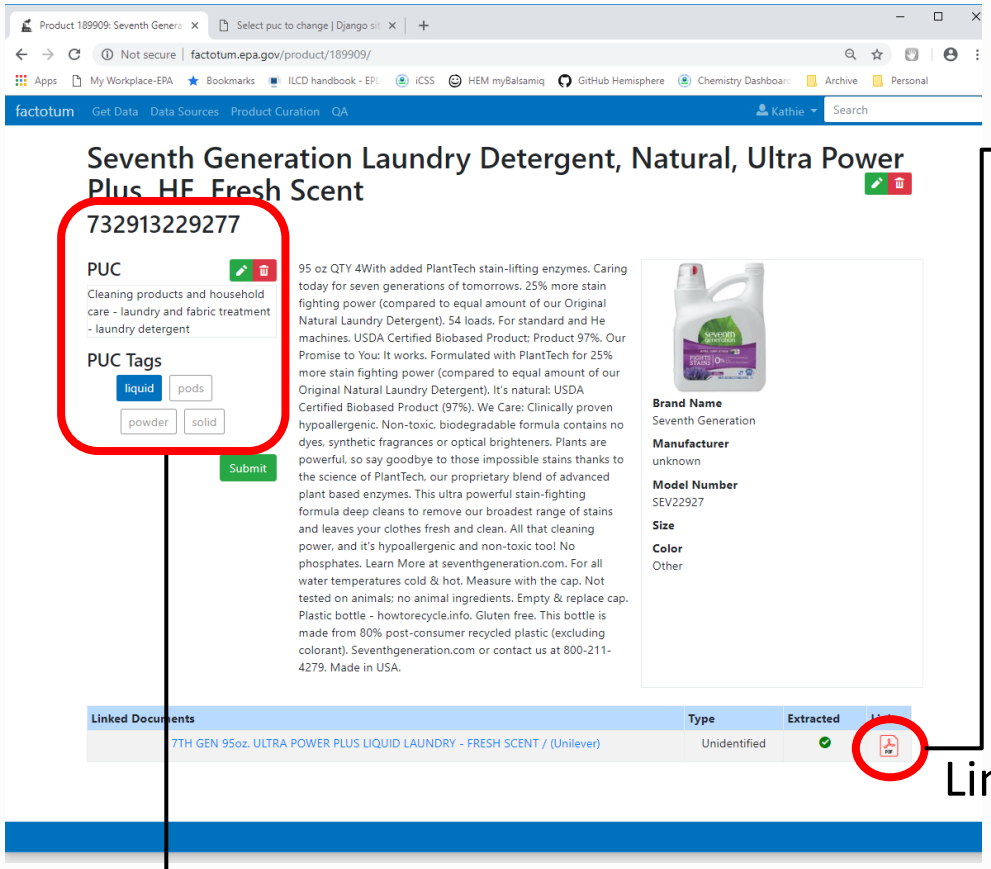
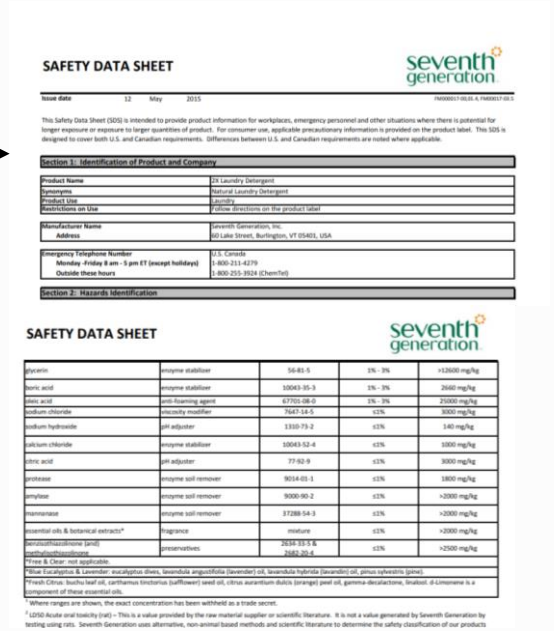
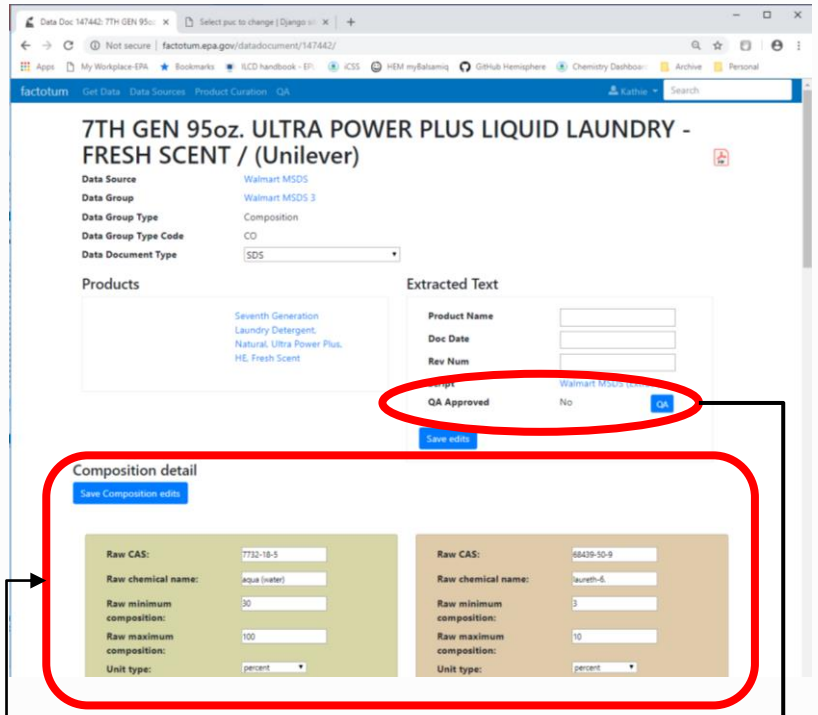


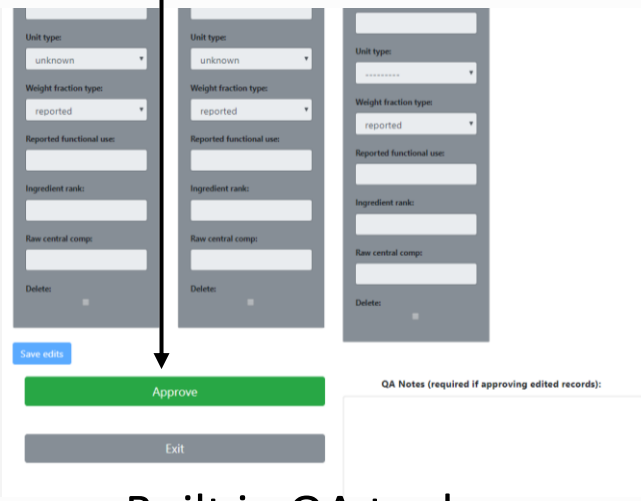
Product UPC & Product category (PUC) assignment



Link to SDS



Extracted composition and functional use data



Built in QA tools

Resulting in improved data quality and availability!

What's next?

Currently available

16,000 products 31,000-58,000 chemicals

- Composition data for formulations
- Functional use data
- Broad categorization of chemical use
- Consumer products assigned to SHEDS-HT product categories (Isaacs et al. 2014)

In progress

>100,000 products ?? chemicals (curation ongoing)

- Increased product scope for composition data
  - Additional product category coverage
  - Building materials and articles
- Revisiting of broad use category terms
- Improved, revised, hierarchical consumer product categories with associated manuscript
- Additional QA
- Additional mapping of chemicals to DTXSID
- Improved ability to update data available on the Dashboard

Acknowledgements

EPA - NCCT
Chris Grulke
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Ann Richard
John Wambaugh (RED)
Antony Williams

EPA - NERL
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David Lyons
Brian Meyer*
Katherine Phillips
Paul Price

*Trainees &
SEE employees

Project Leads

CSRA, under contract to the EPA, provides direct development support for the CPDat data management tool.

Visit the CompTox Chemicals Dashboard to explore our data:
https://comptox.epa.gov/dashboard

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