United States Environmental Protection Agency

The Chemical and Products Database (CPDat)

Kathie Dionisio, Katherine Phillips, Kristin Isaacs

U.S. Environmental Protection Agency, Office of Research and Development
National Exposure Research Laboratory

Computational Toxicology Communities of Practice
October 25, 2018

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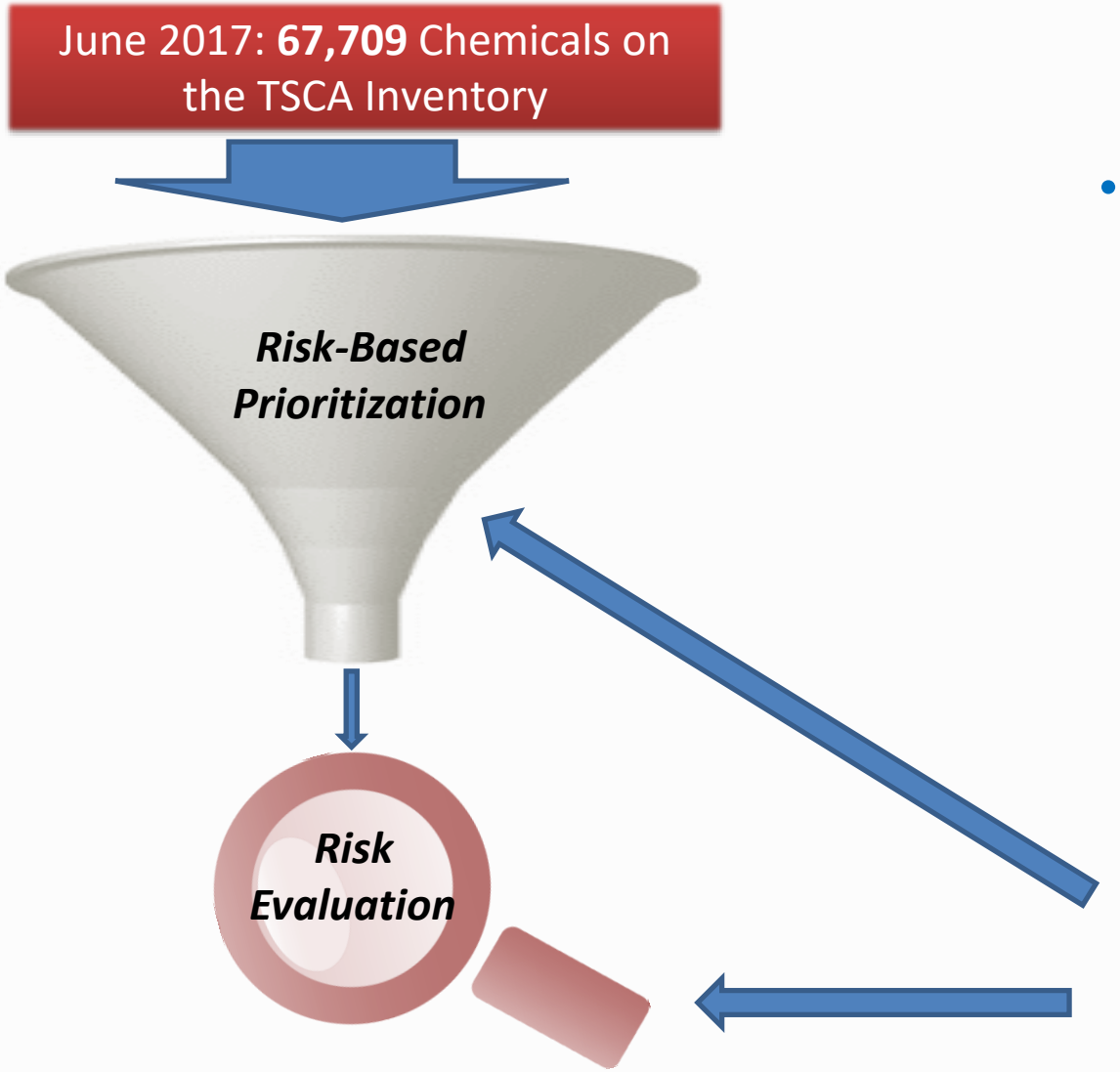
TSCA and the need for exposure information



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

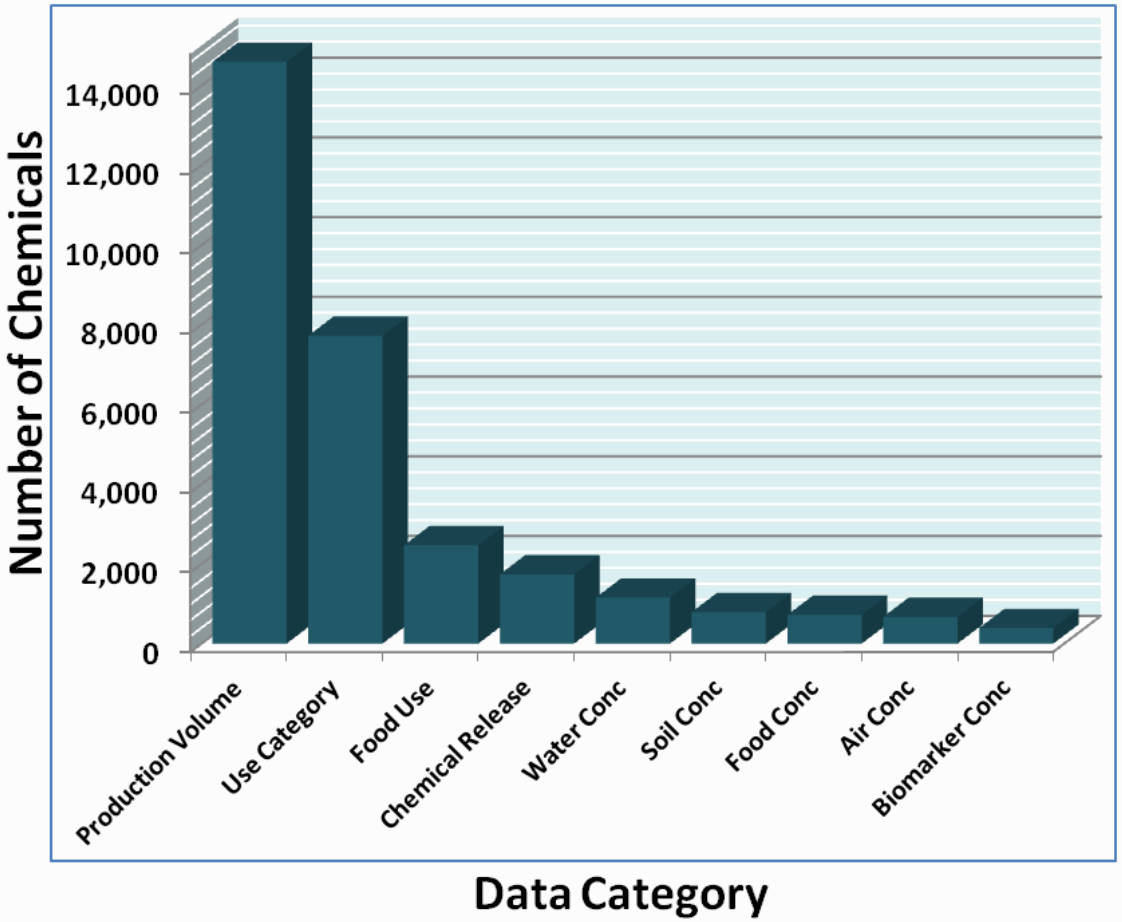
- Amends the Toxic Substances Control Act (TSCA)
  - Mandatory requirement for EPA to evaluate existing chemicals with clear and enforceable deadlines
  - Risk-based chemical assessments
  - Increased public transparency for chemical information

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)

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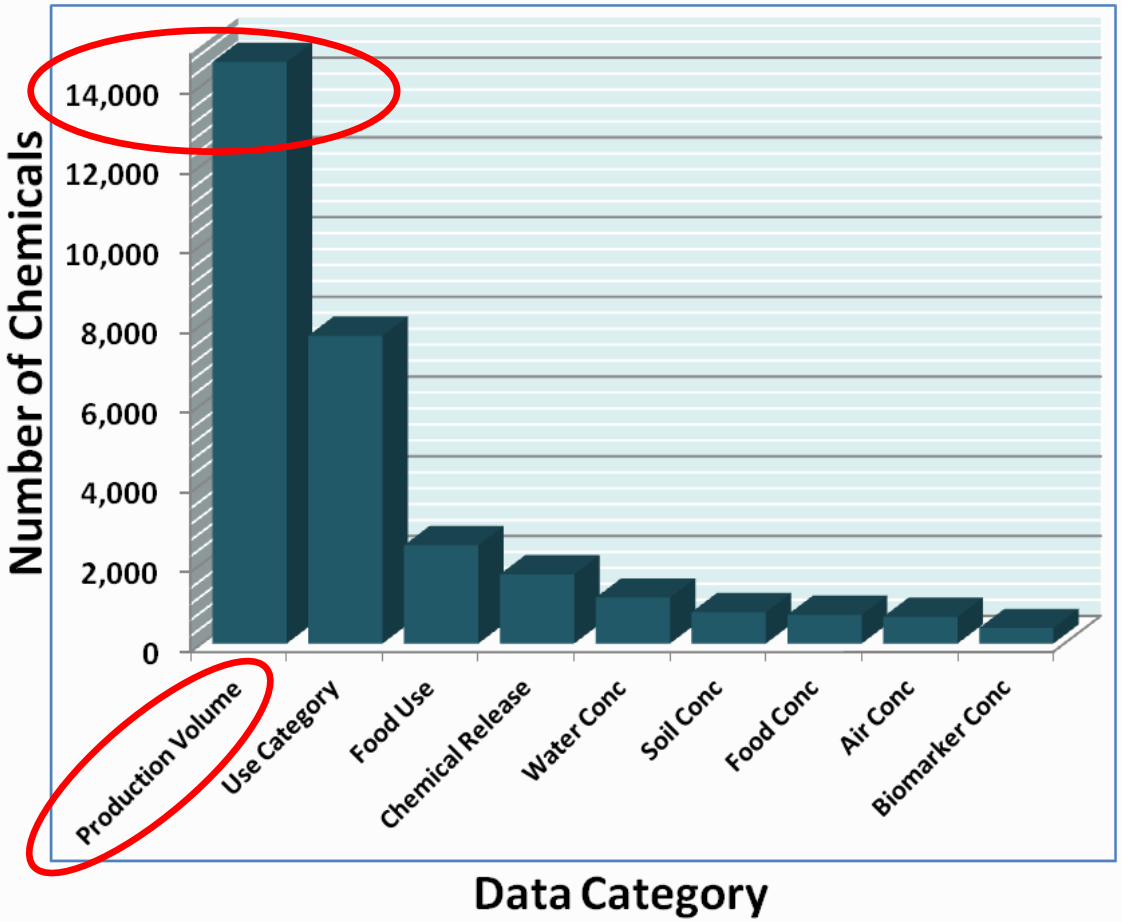

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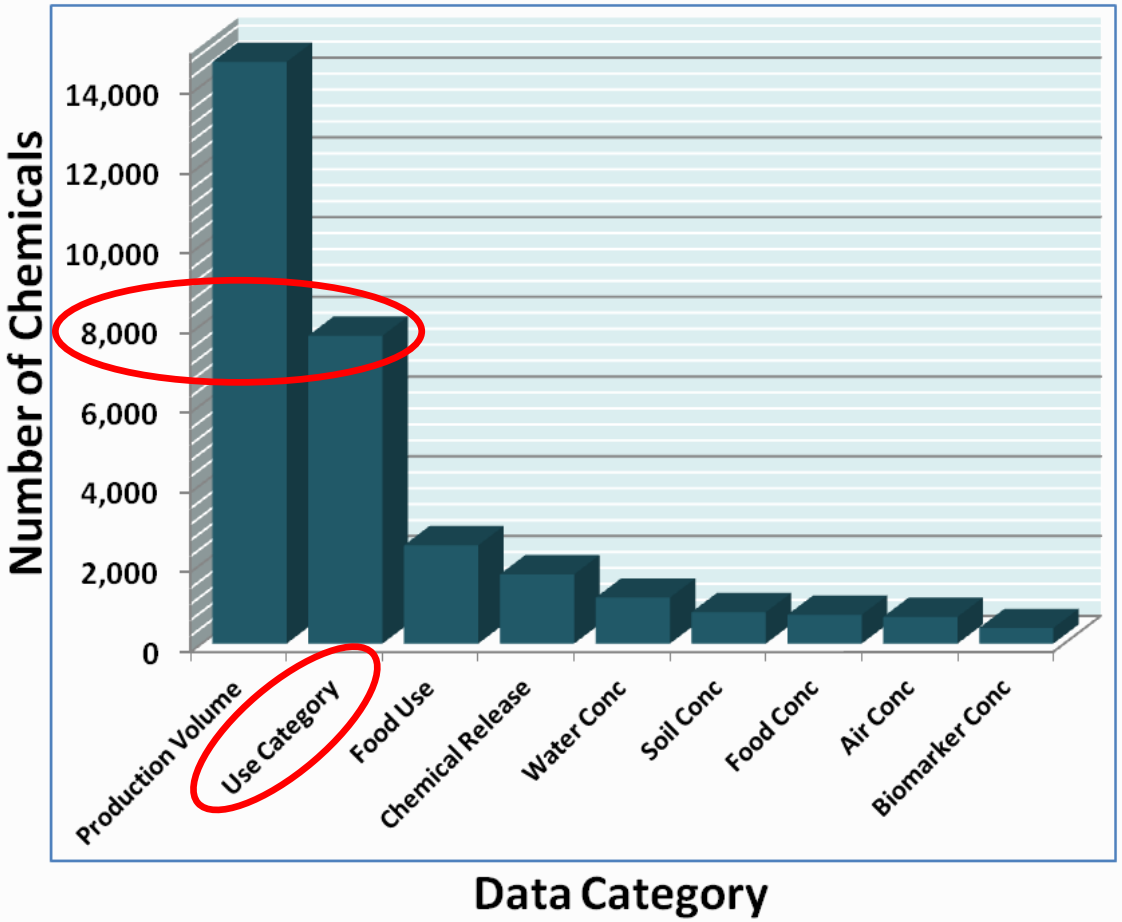


Egeghy et al. *Science of the Total Environment* (2012)

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

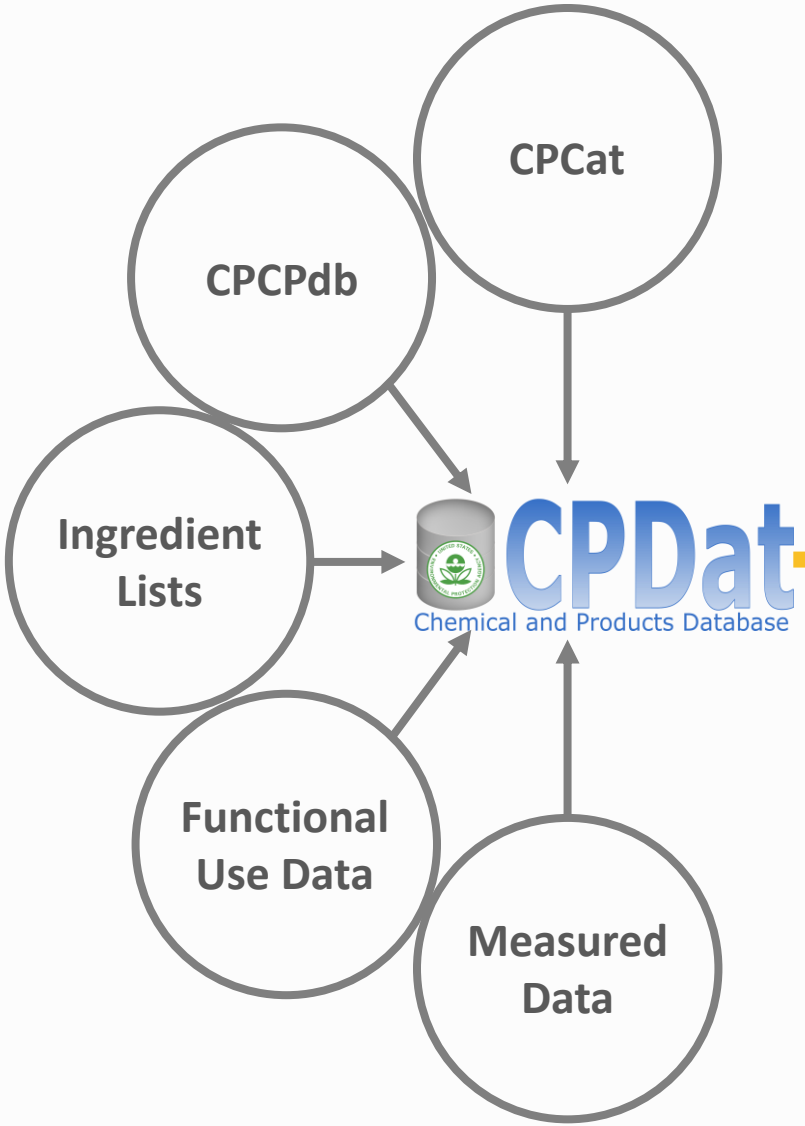
The Chemicals and Products Database (CPDat)

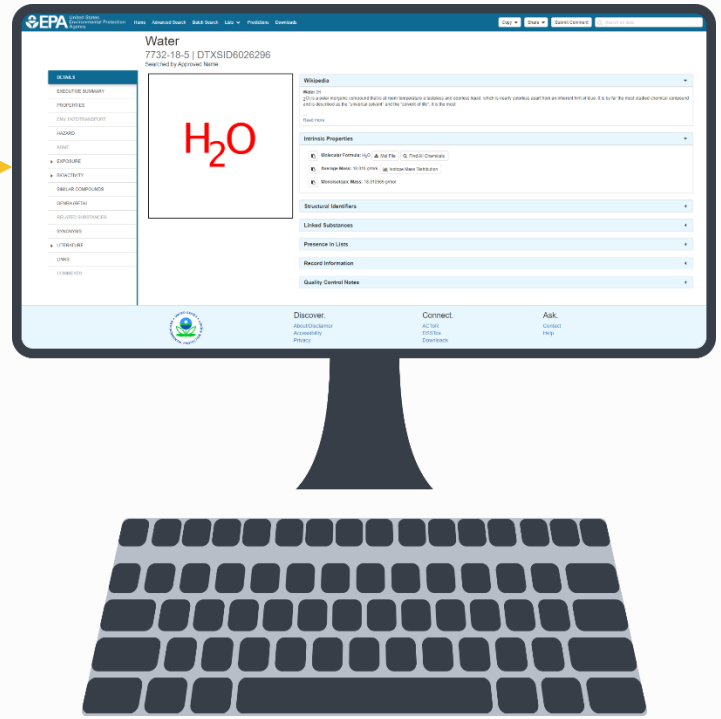
- Provides a means to organize and disseminate chemical and product information
- Comprised of chemical use and consumer product composition data from a variety of public sources; includes measured, modeled, and reported data
- Organized around a set of consumer product use categories (PUCs) optimized 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

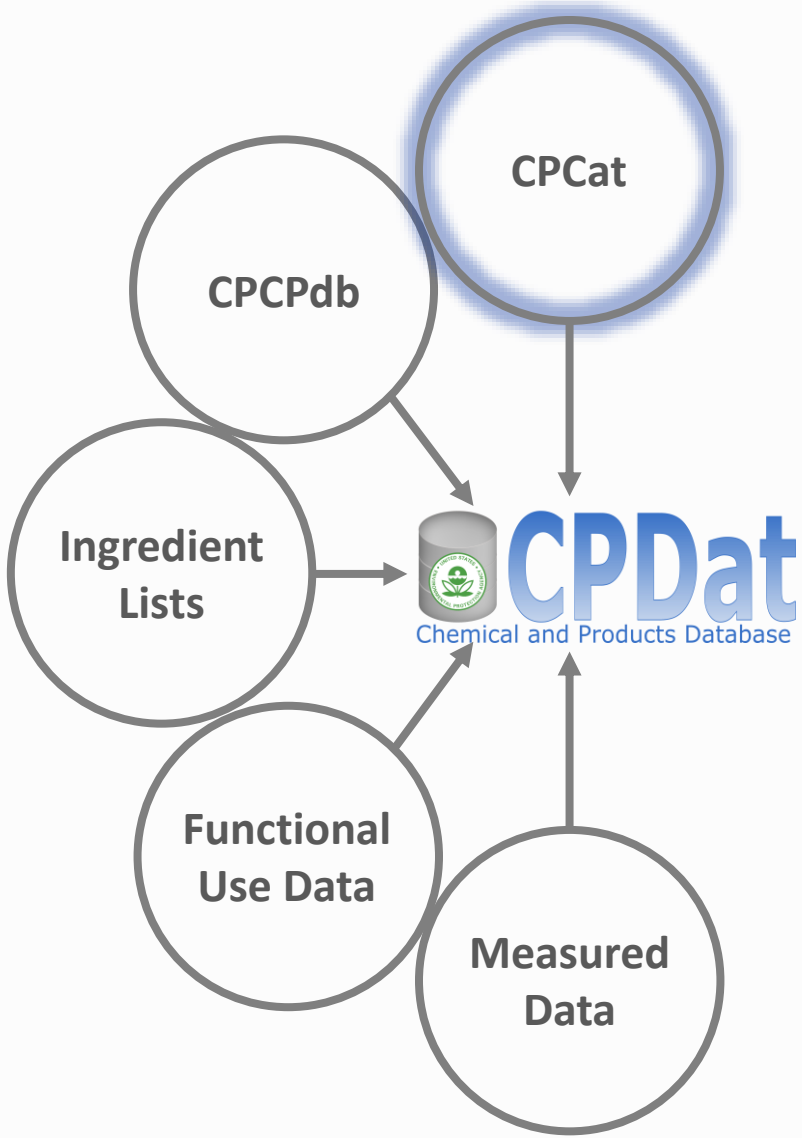
What is CPDat?

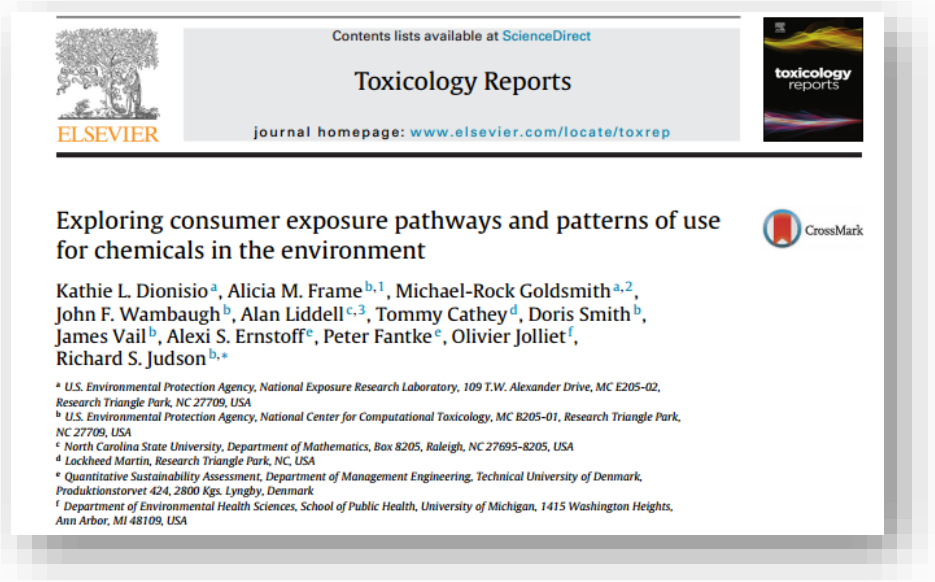




https://comptox.epa.gov/dashboard

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

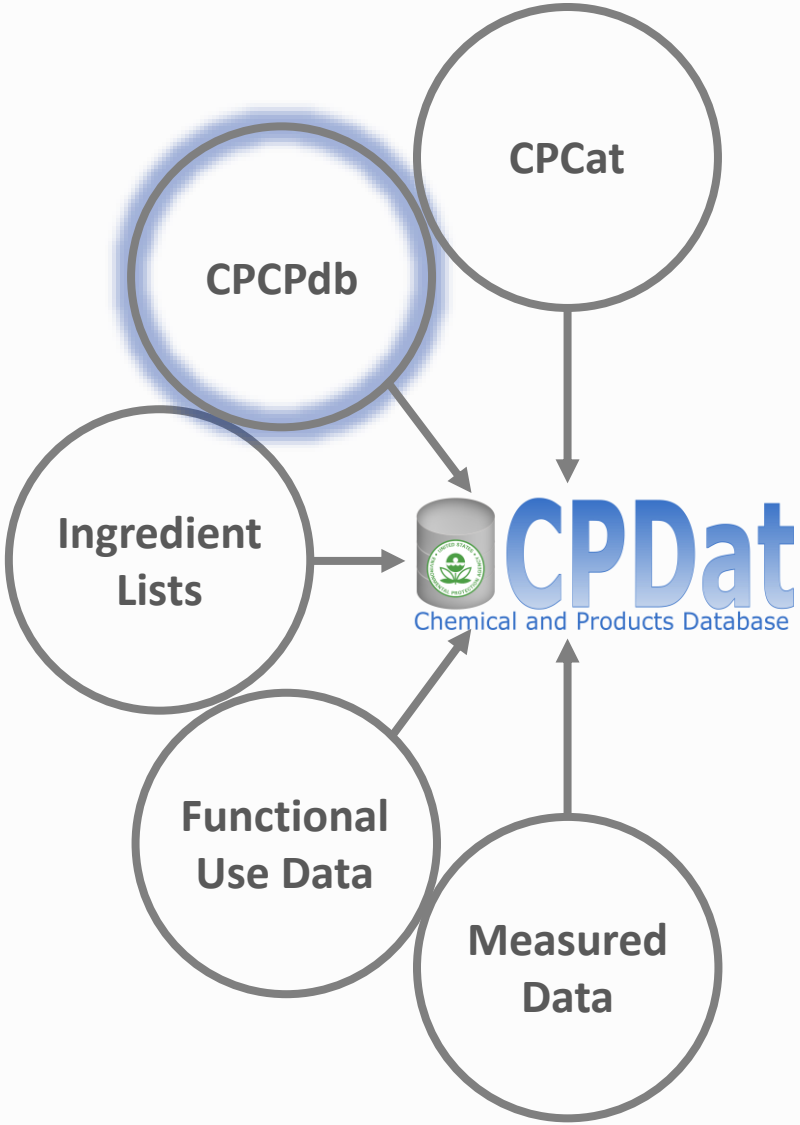
Kathie L. Dionisio[a], Alicia M. Frame[b,1], Michael-Rock Goldsmith[a,2], John F. Wambaugh[b], Alan Liddell[c,3], Tommy Cathey[d], Doris Smith[b], James Vail[b], Alexi S. Ernstoff[e], Peter Fantke[e], Olivier Jolliet[f], Richard S. Judson[b,*]

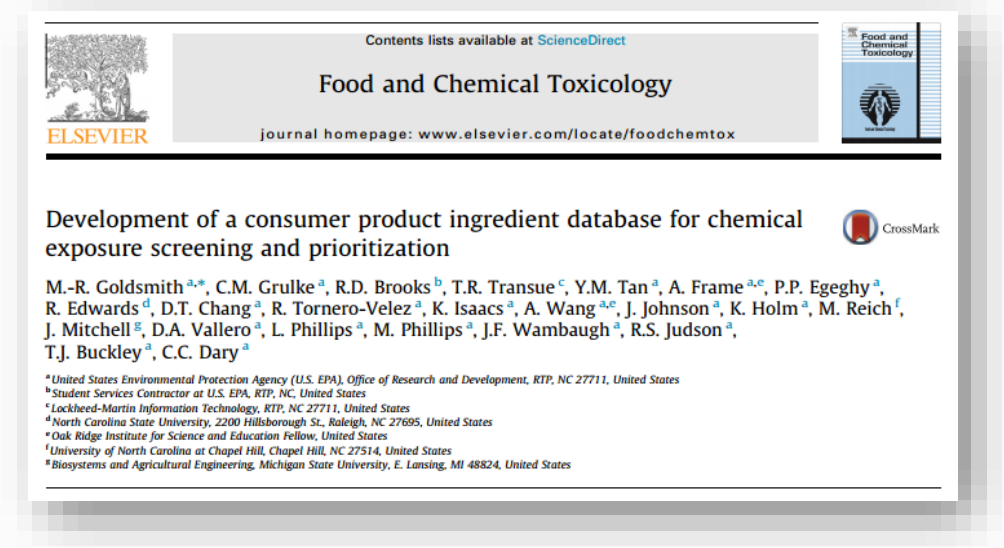
[a] U.S. Environmental Protection Agency, National Exposure Research Laboratory, 109 T.W. Alexander Drive, MC E205-02, Research Triangle Park, NC 27709, USA
[b] U.S. Environmental Protection Agency, National Center for Computational Toxicology, MC B205-01, Research Triangle Park, NC 27709, USA
[c] North 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?





Contents lists available at ScienceDirect

Food and Chemical Toxicology

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

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

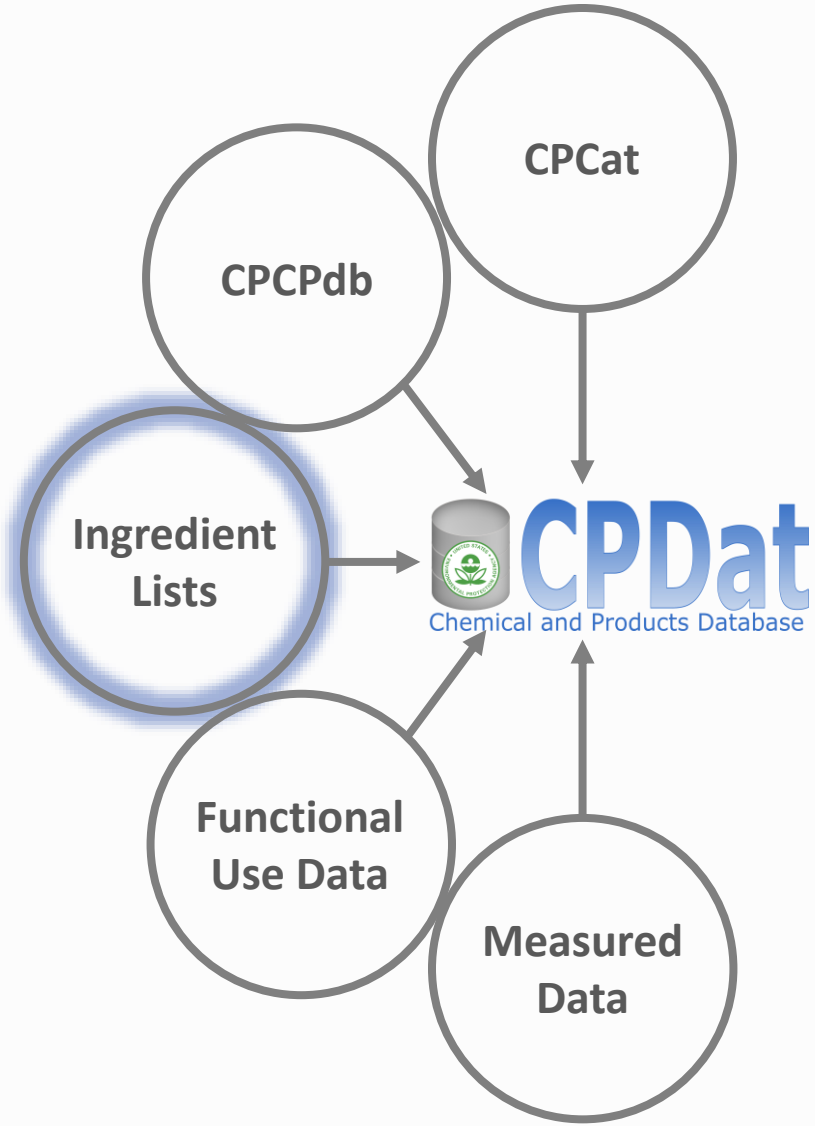
M.-R. Goldsmith [a,*], C.M. Grulke [a], R.D. Brooks [b], T.R. Transue [c], Y.M. Tan [a], A. Frame [a,e], P.P. Egeghy [a], R. Edwards [d], D.T. Chang [a], R. Tornero-Velez [a], K. Isaacs [a], A. Wang [a,e], J. Johnson [a], K. Holm [a], M. Reich [f], J. Mitchell [g], D.A. Vallero [a], L. Phillips [a], 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
[e] Oak Ridge Institute for Science and Education Fellow, United States
[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
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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

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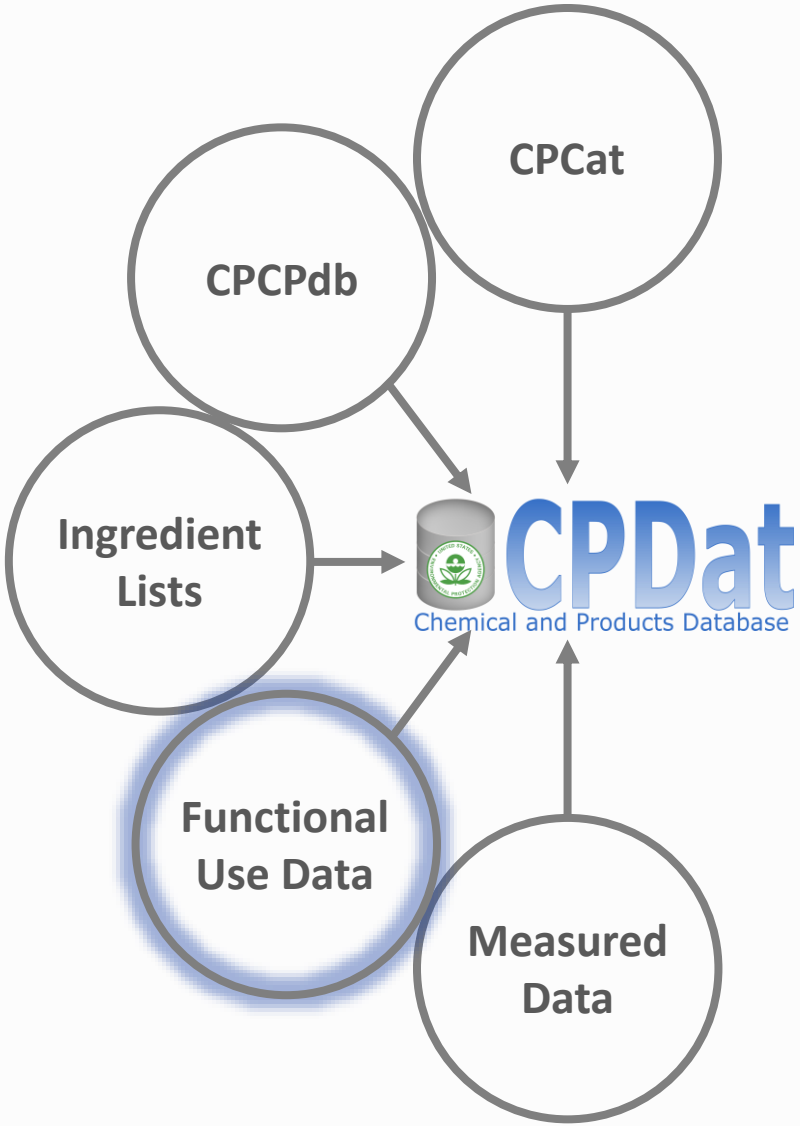

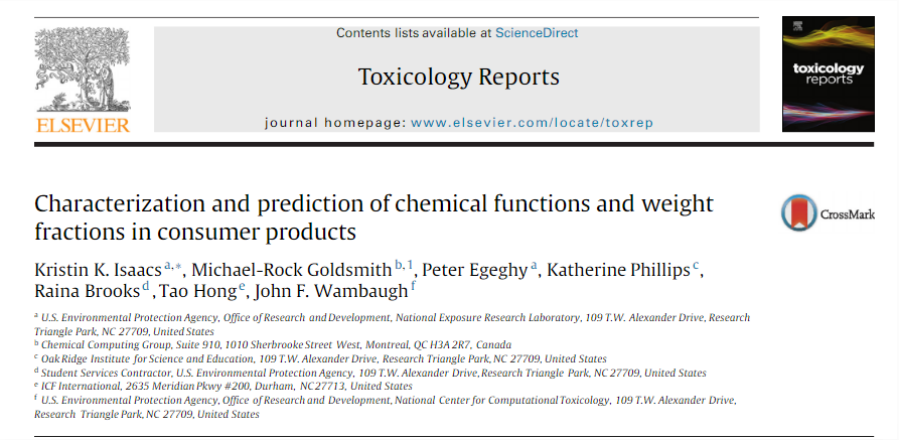

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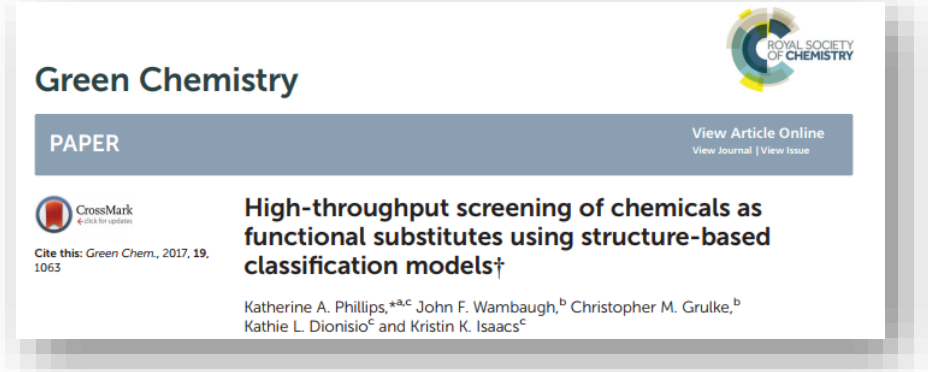
Toxicology Reports

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

View Article Online
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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

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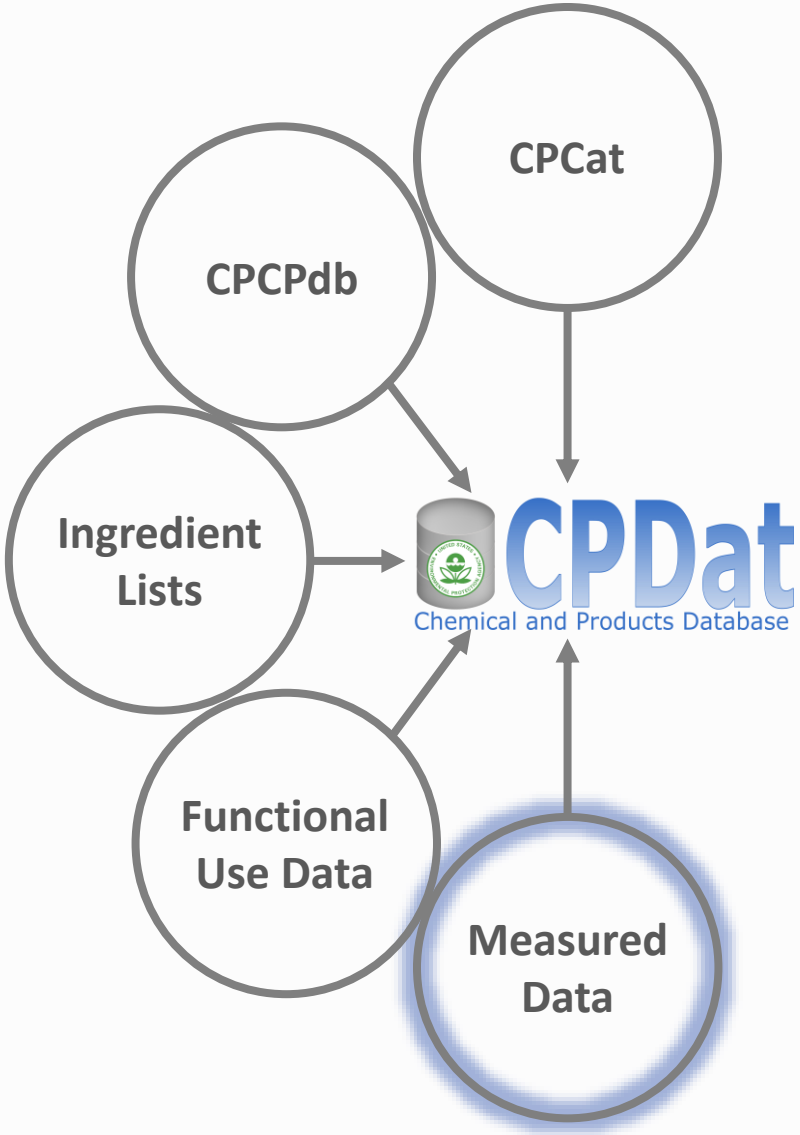
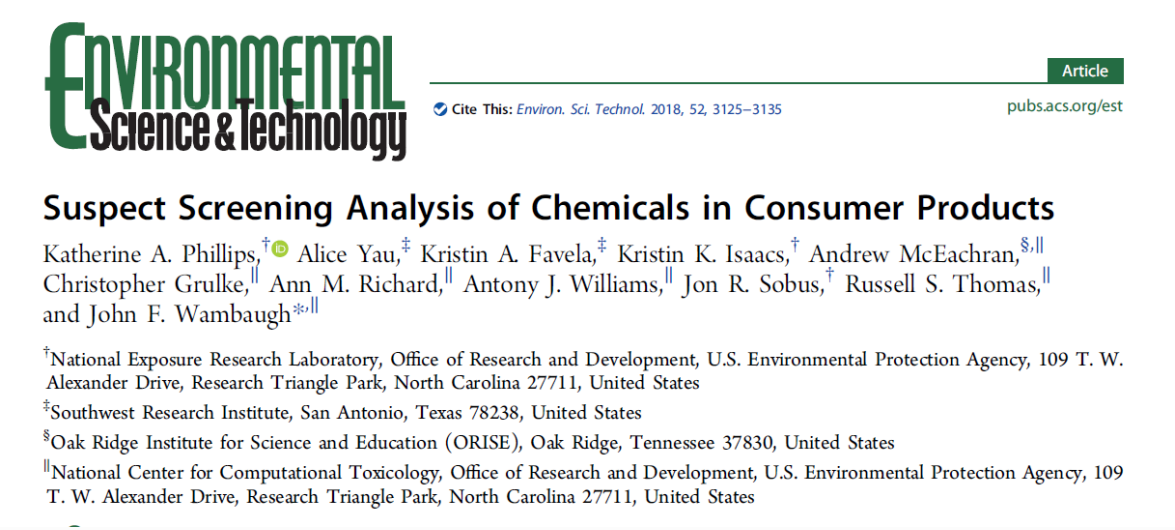




Environmental Science & Technology
Article
Cite This: Environ. Sci. Technol. 2018, 52, 3125−3135
pubs.acs.org/est

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*[,∥]

[†]National Exposure Research Laboratory, Office of Research and Development, U.S. Environmental Protection Agency, 109 T. W. Alexander Drive, Research Triangle Park, North Carolina 27711, United States

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

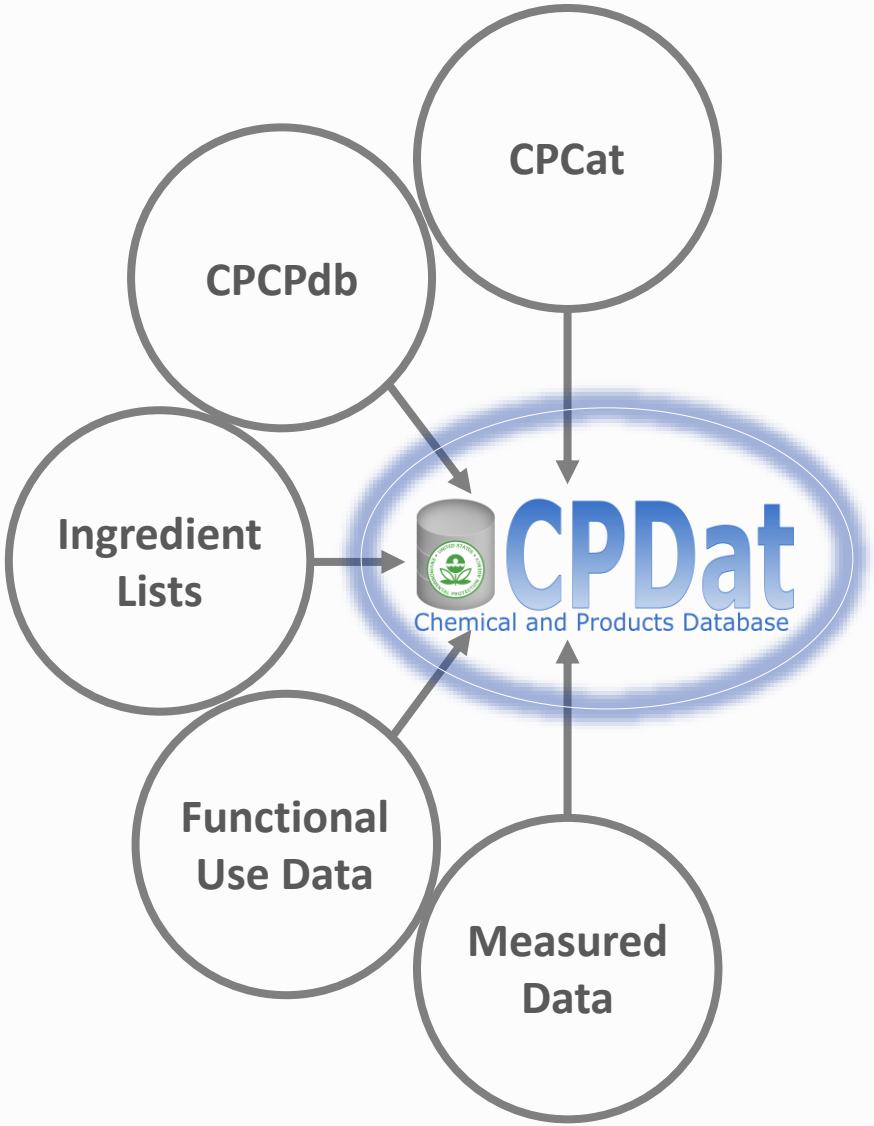
[§]Oak Ridge Institute for Science and Education (ORISE), Oak Ridge, Tennessee 37830, United States

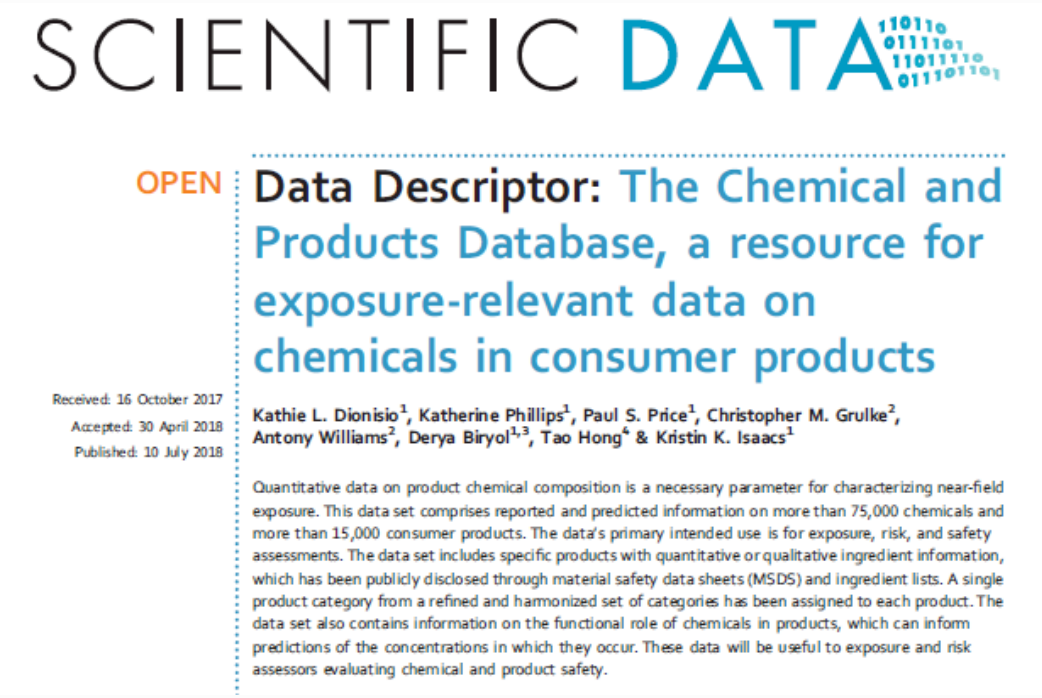
[∥]National Center for Computational Toxicology, Office of Research and Development, U.S. Environmental Protection Agency, 109 T. W. Alexander Drive, Research Triangle Park, North Carolina 27711, United States

Targeted and non-targeted measurement of chemicals in consumer products

- Measured weight fractions
- Confirmed presence
- Tentative identification

What is CPDat?





SCIENTIFIC DATA

OPEN

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

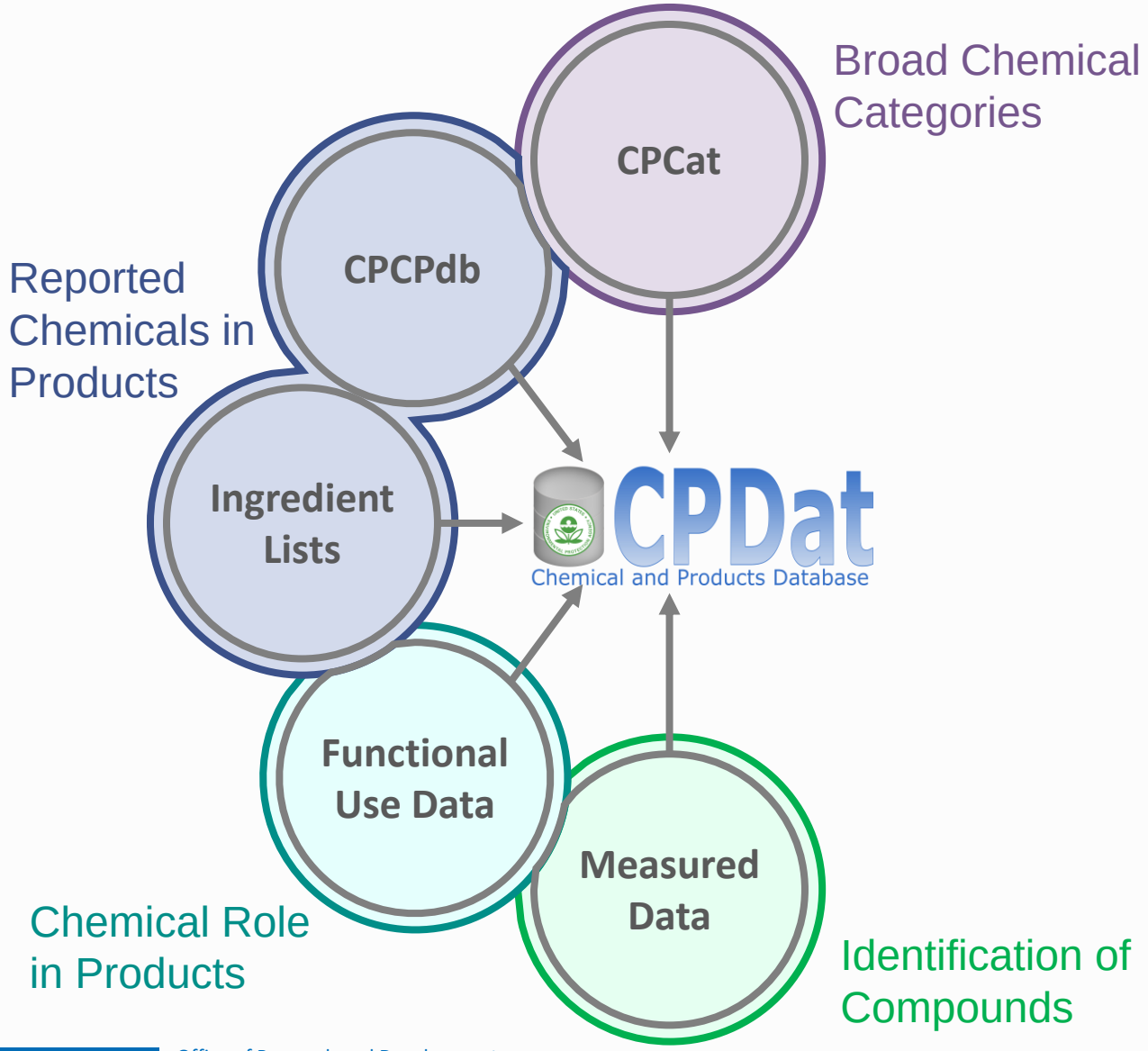
Received: 16 October 2017
Accepted: 30 April 2018
Published: 10 July 2018

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?

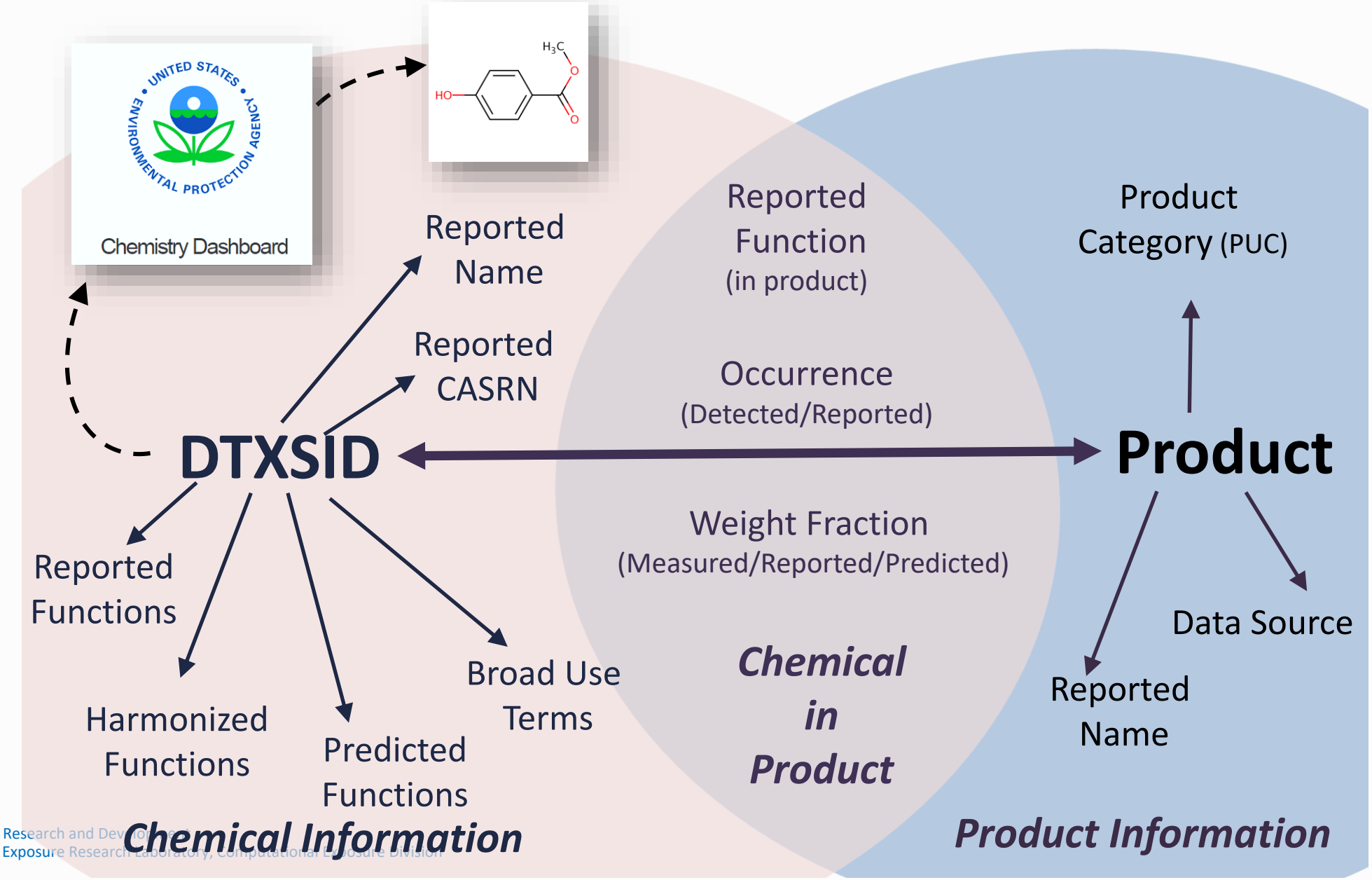


30,000-60,000 chemicals

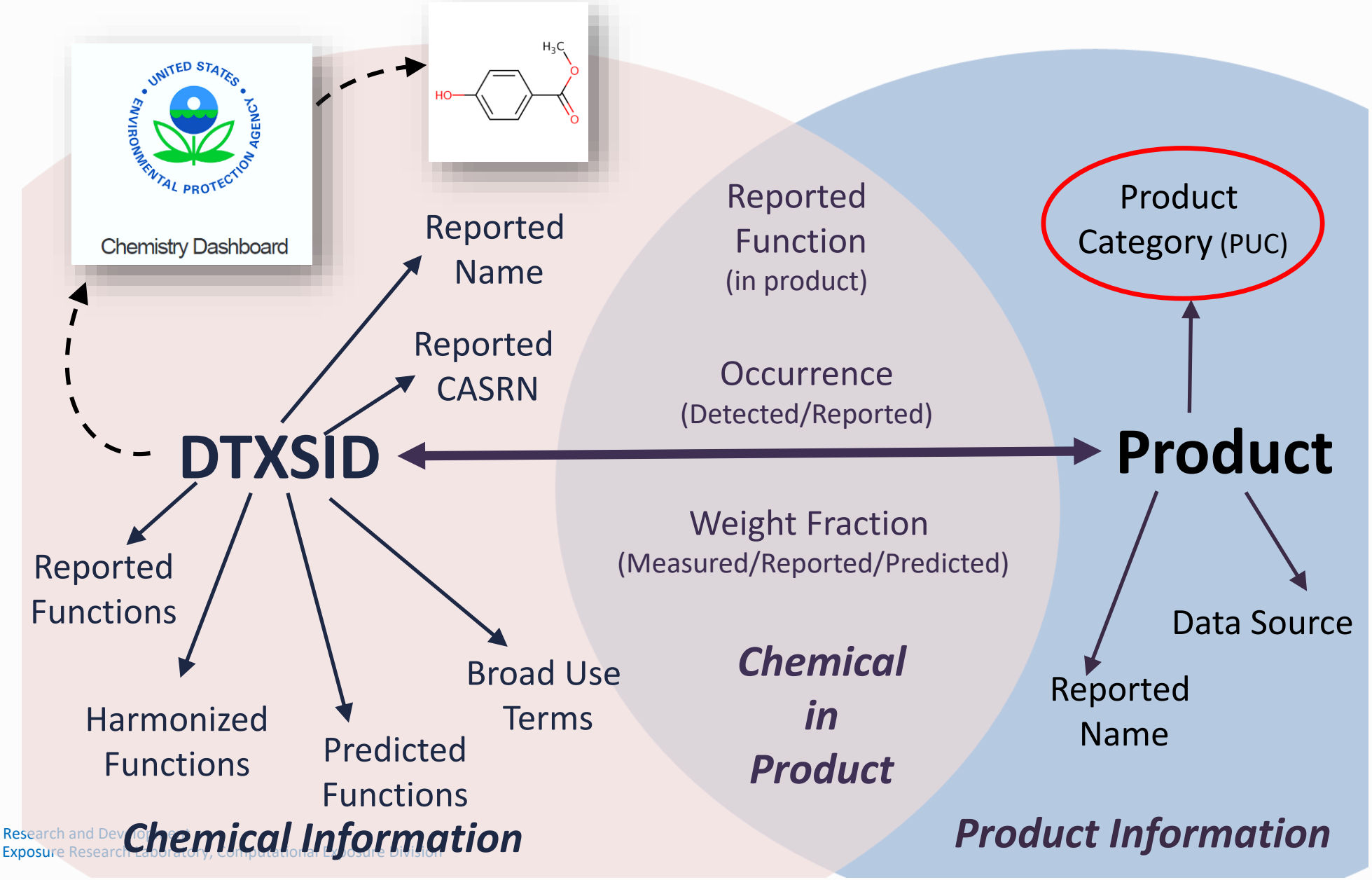
16,000 products

~200 consumer product categories

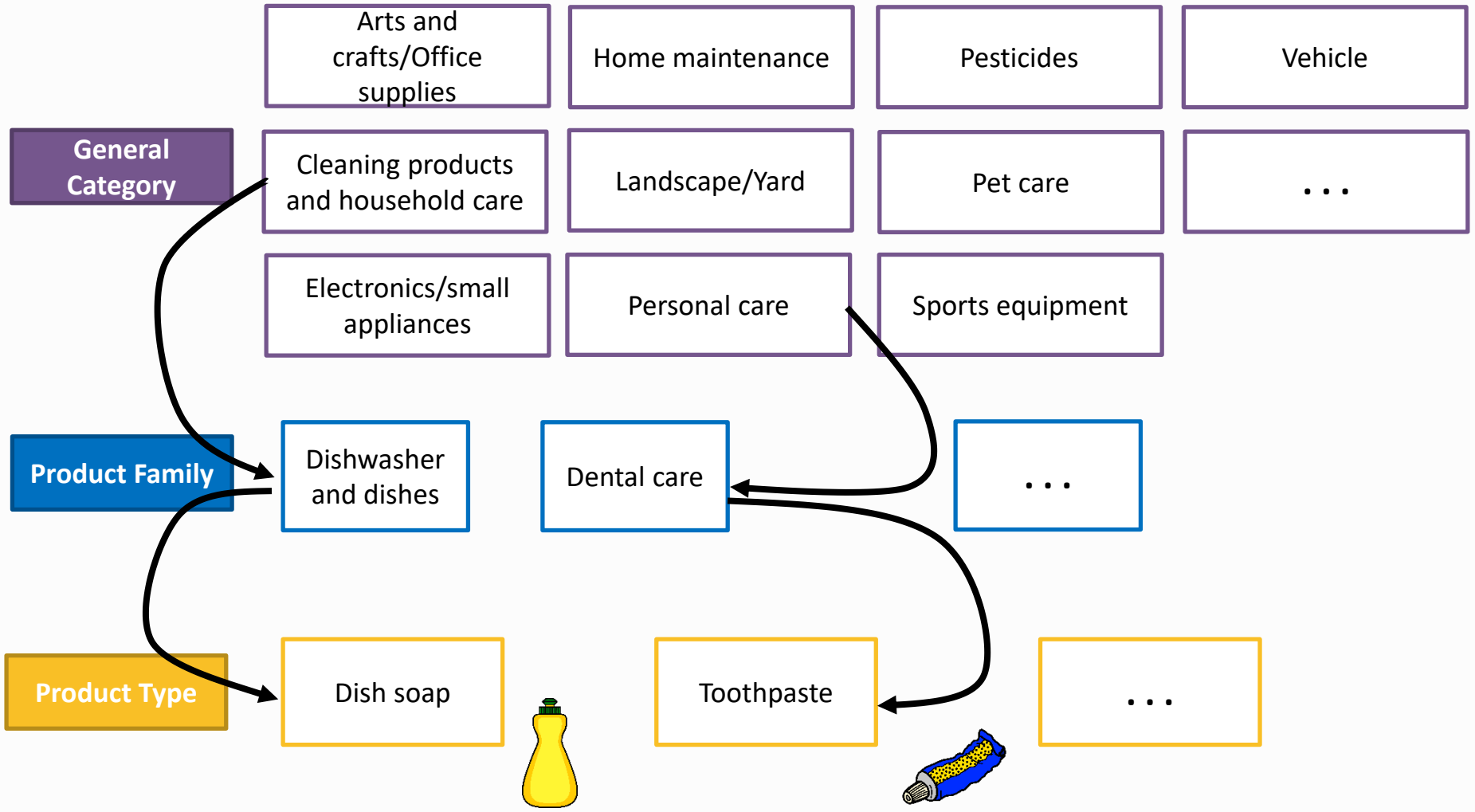
Information linkages in CPDat



Information linkages in CPDat

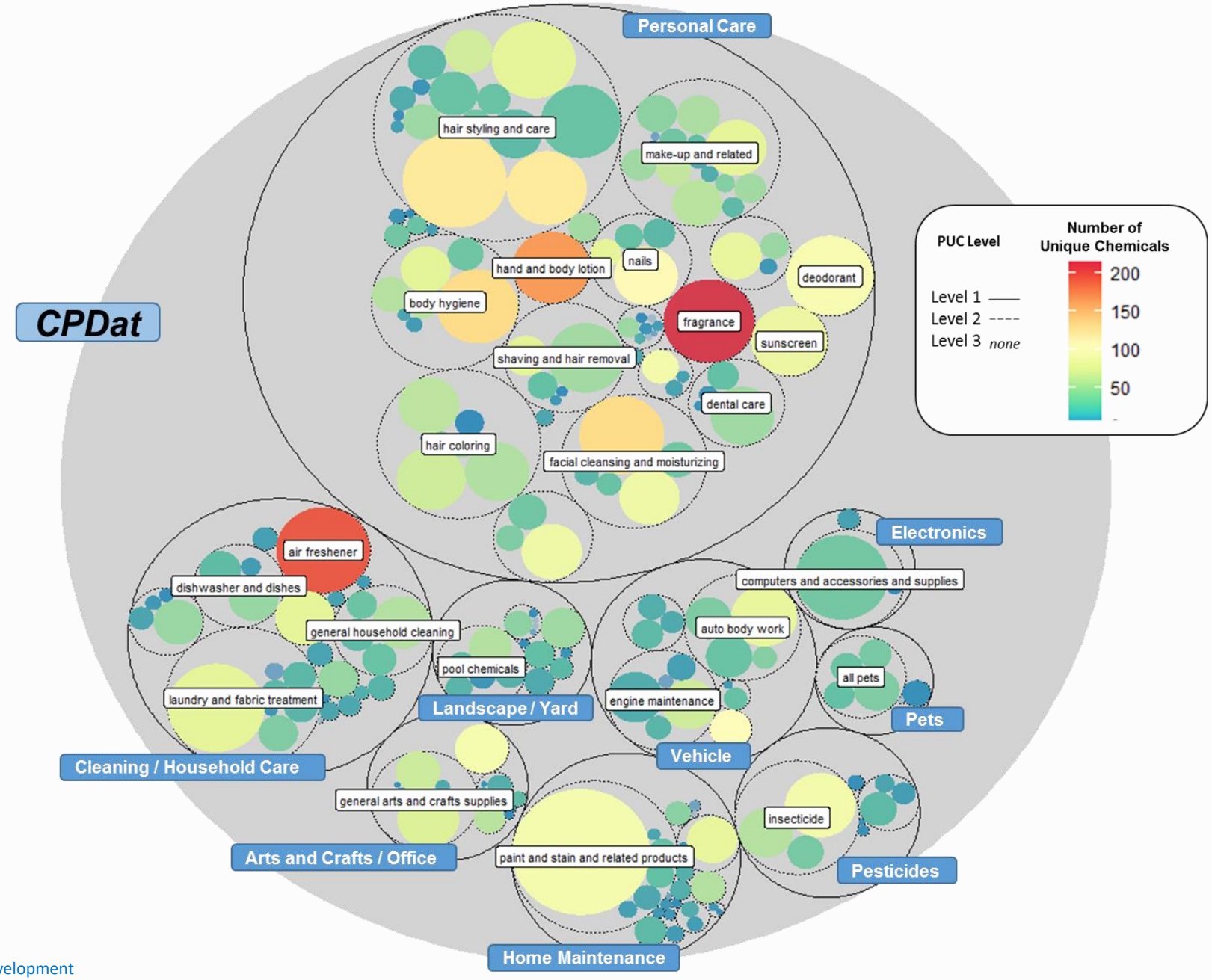


Product Use Categories (PUCs) in CPDat

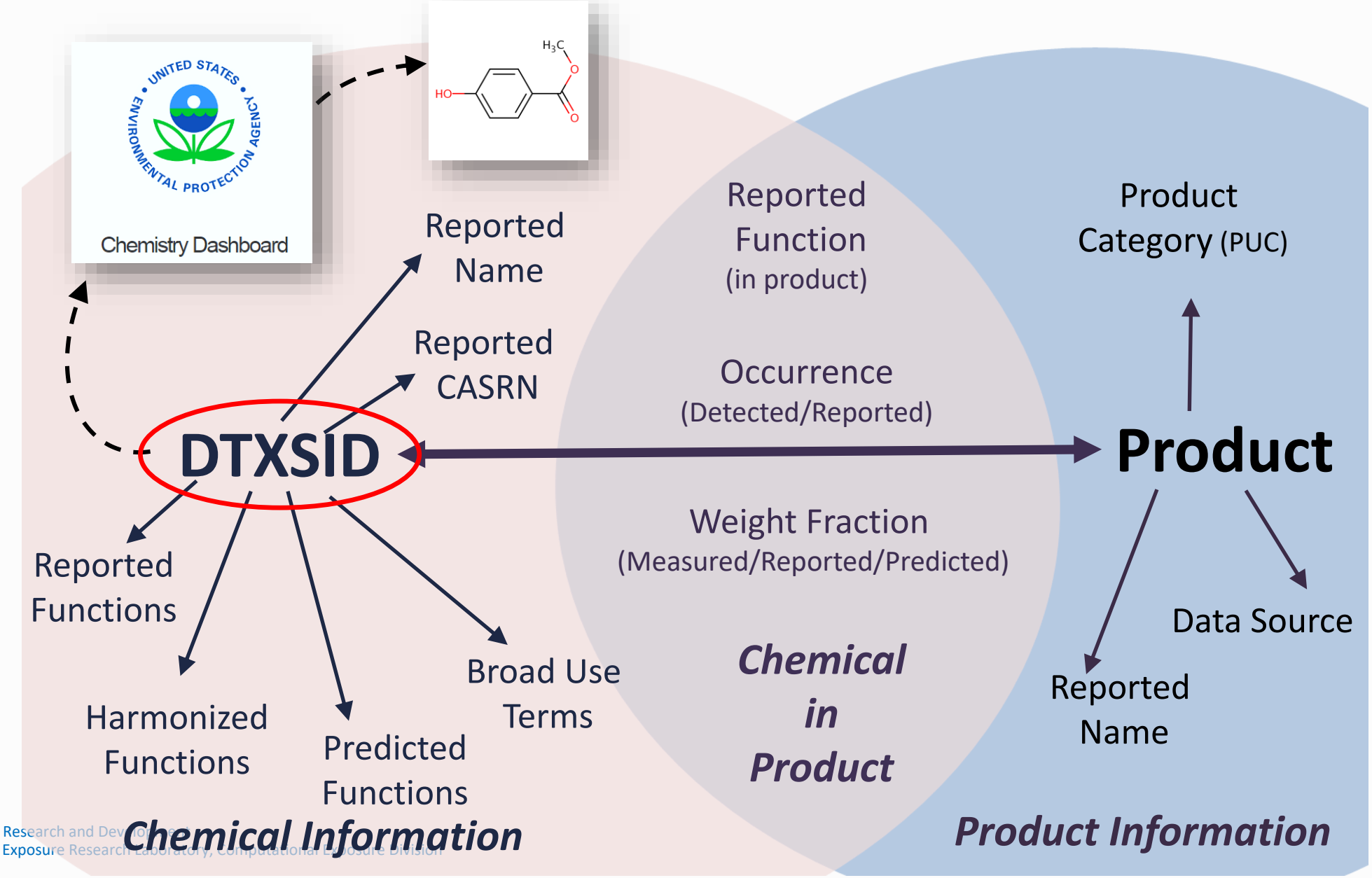


- PUCs group products based on
  - Meeting a common need
  - Having similar routes of exposures
- PUCs are consistent with harmonized OECD system of product categorizations for chemical reporting
- Hierarchy based system

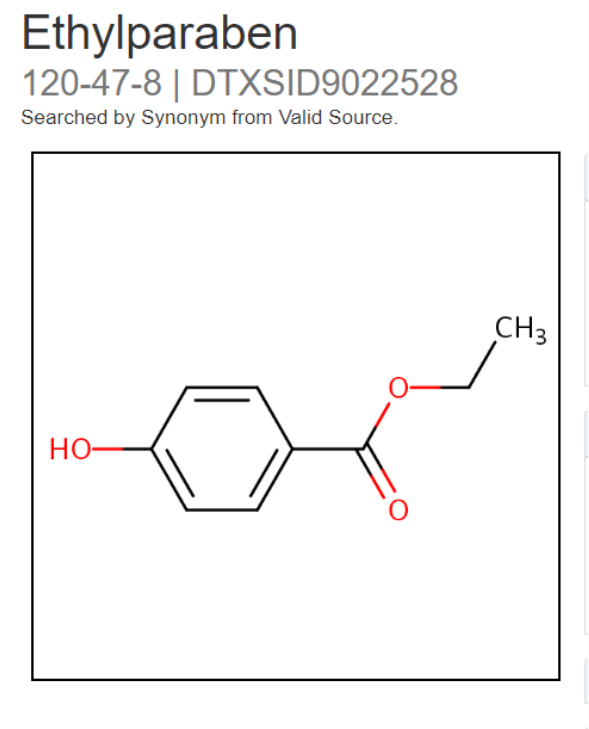
United States
Environmental Protection
Agency



Information linkages in CPDat



Chemical identification

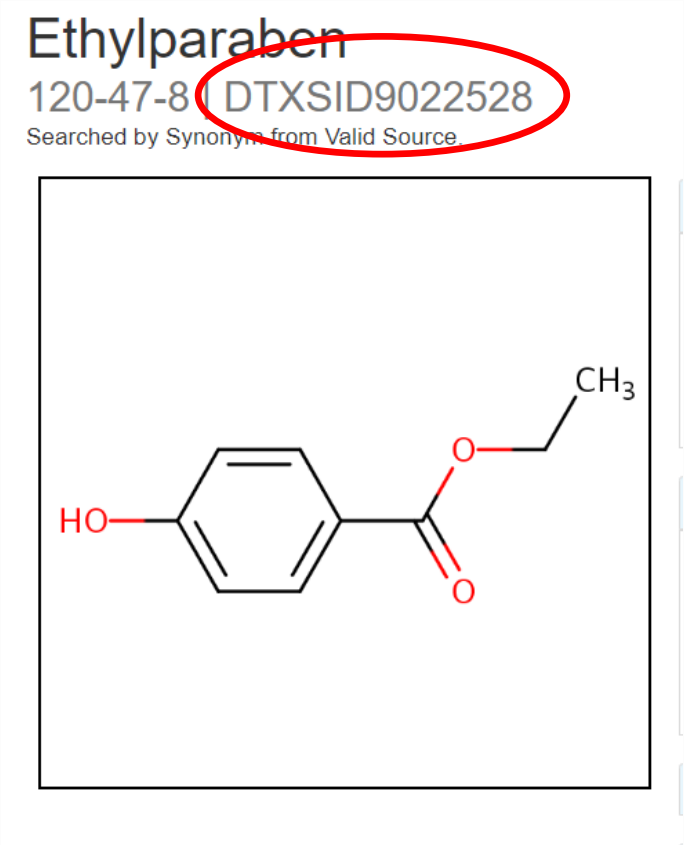


Correct chemical identification is important (and difficult!)

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

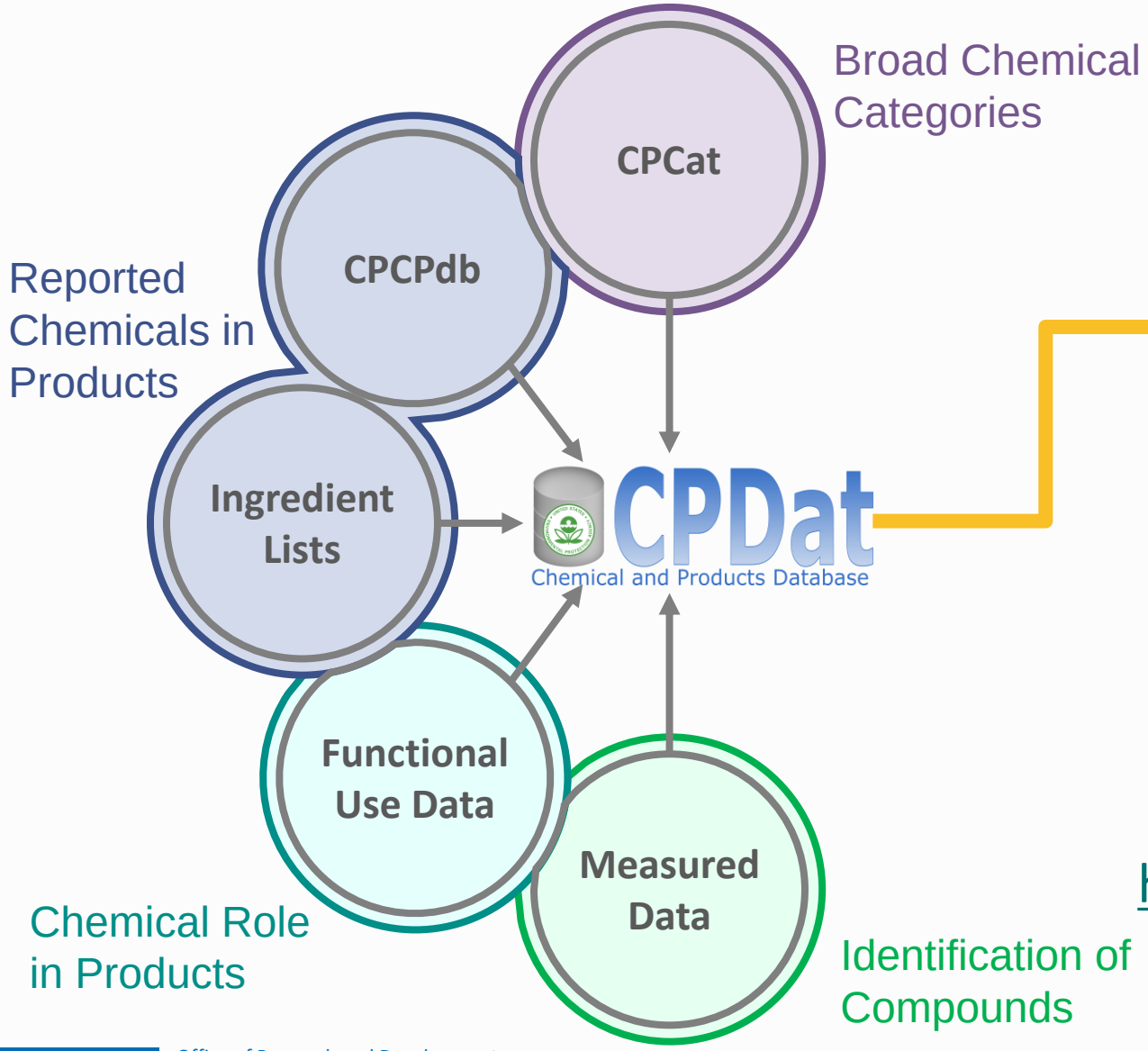
49,000 unique CAS

68,000 unique chemical names

31,000 unique substances (by DTXSID)

(+27,000 substances not yet curated)

How to access CPDat?

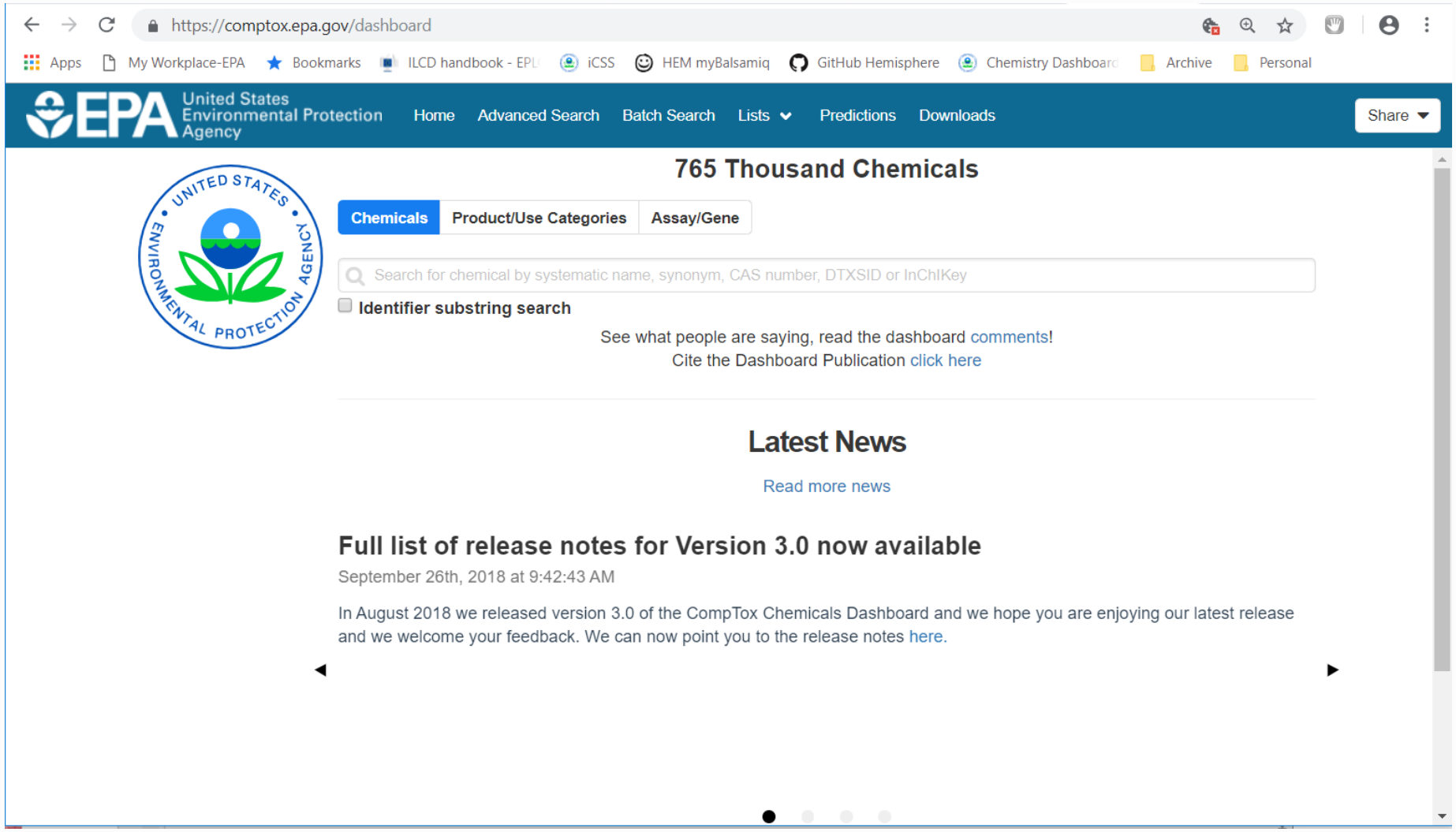


Williams et al., *J. Cheminfo.*, 2017

Freely search, explore, and use our data

https://comptox.epa.gov/dashboard

How to access CPDat?



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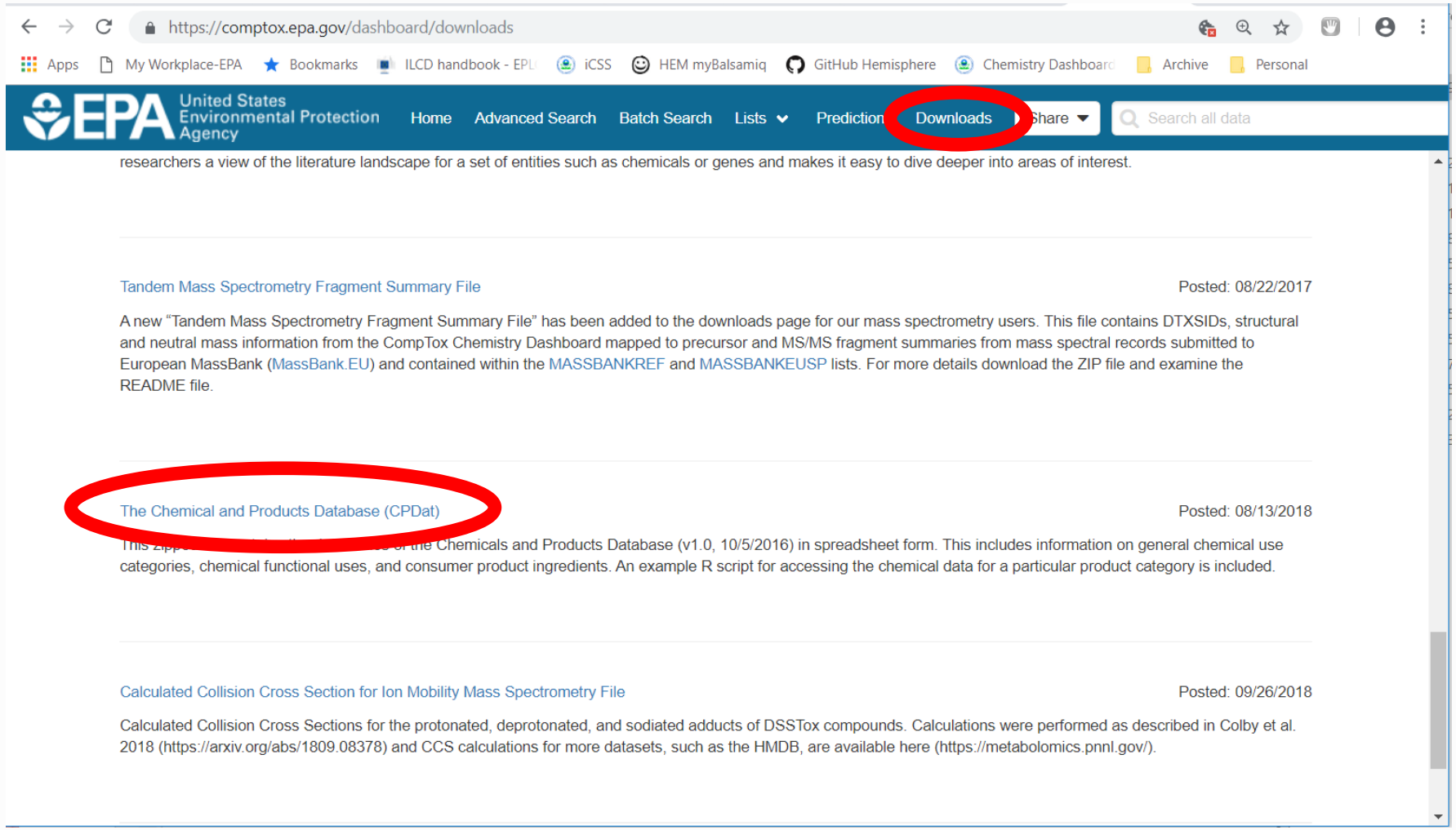

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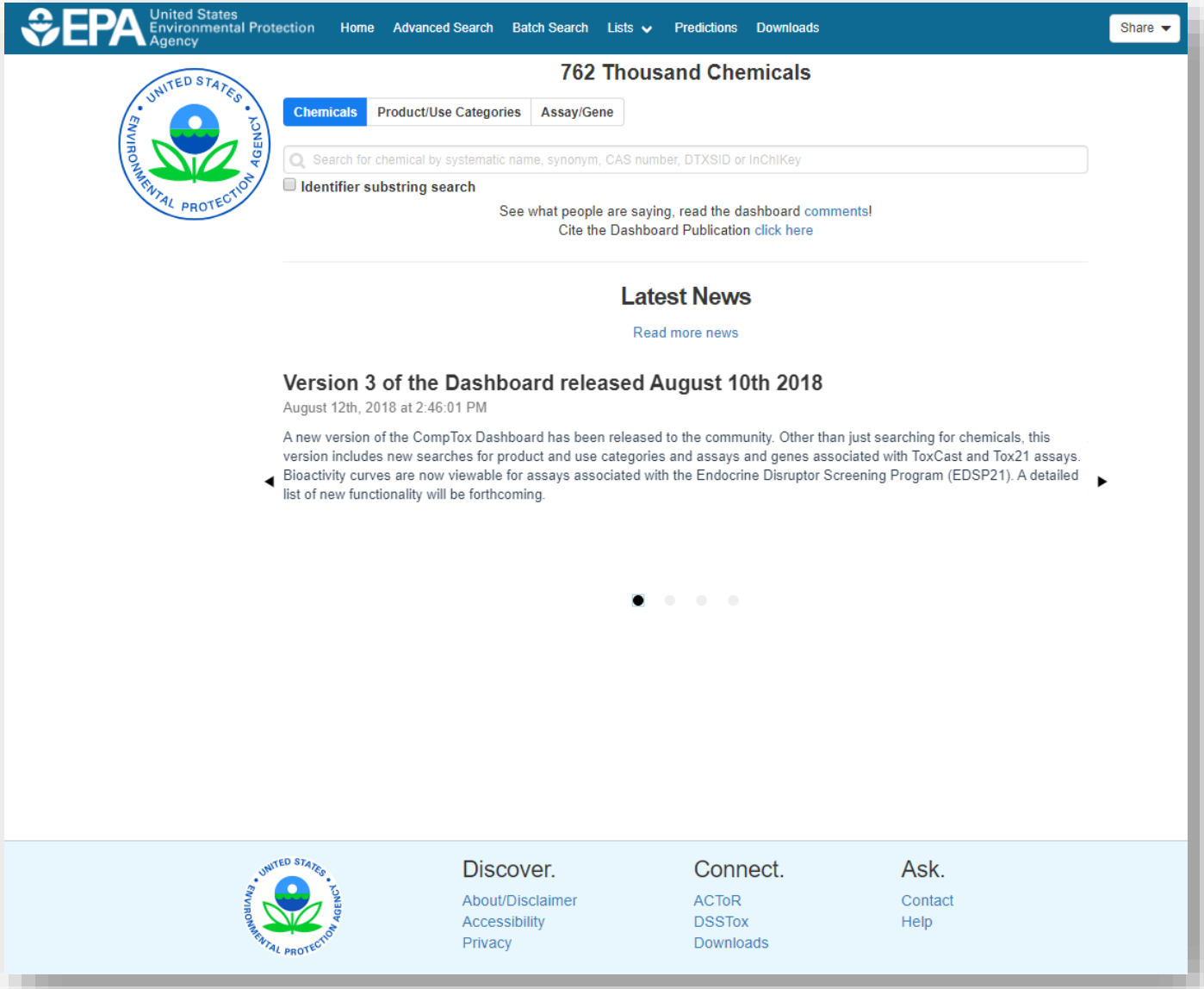
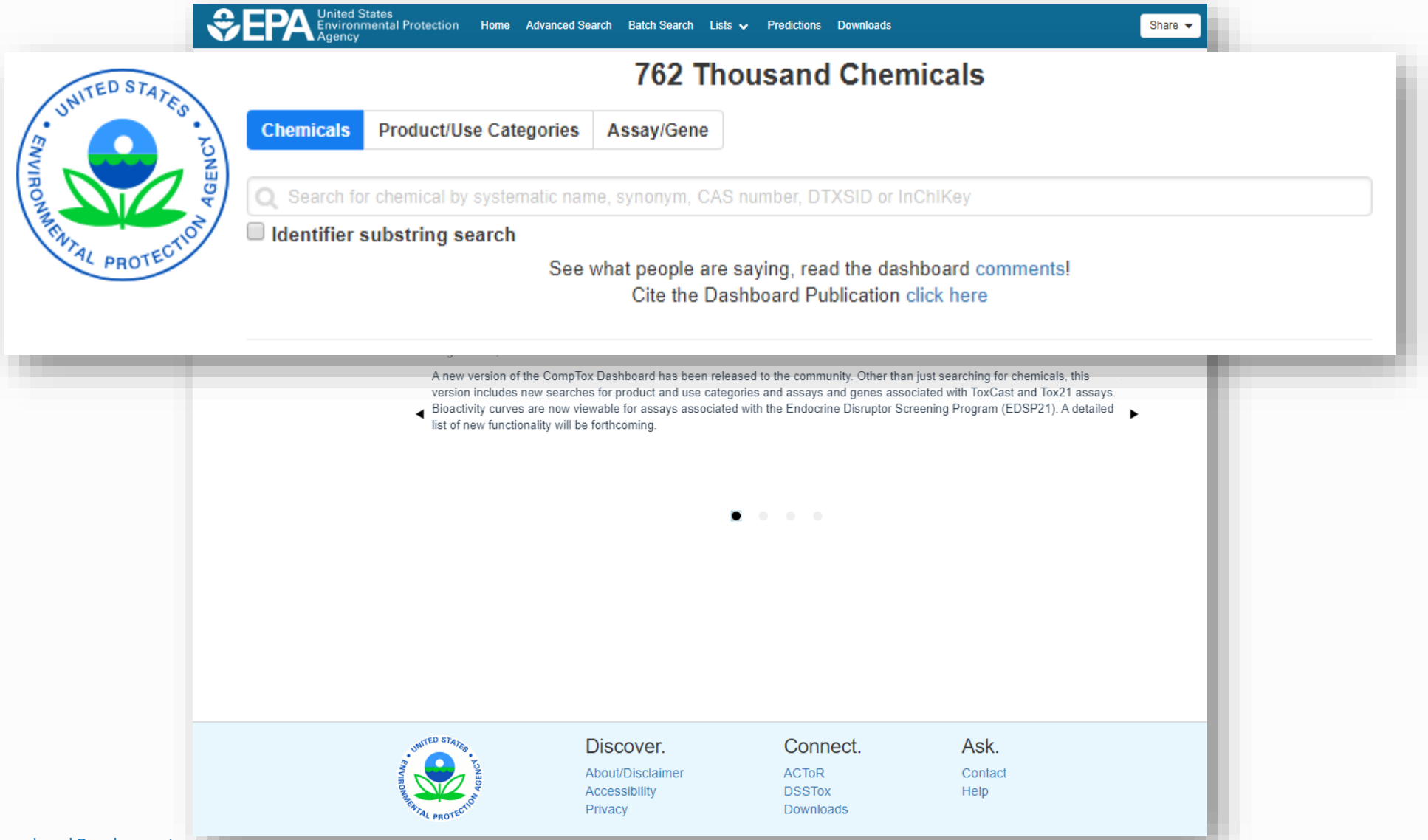
Using the CompTox Chemicals Dashboard to access CPDat



Searching by chemical



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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
- Hexadecanoic acid, (3,5-dioxo-4-(3-oxo-3-phenylpropyl)-1,2-diphenyl-4-pyrazolidinyl)methyl ester
  DTXSID90195015
- Hexadecanoic acid, (3,5-dioxo-4-(3-oxobutyl)-1,2-diphenyl-4-pyrazolidinyl)methyl ester
  DTXSID10195012

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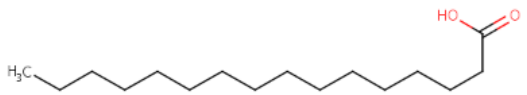
Hexadecanoic acid

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



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 $CH_3(CH_2)_{14}COOH$, 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: $C_{16}H_{32}O_2$

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

United States Environmental Protection Agency

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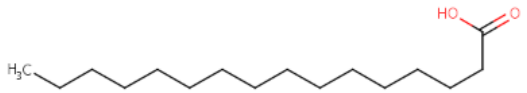
Hexadecanoic acid

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



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Hexadecanoic acid

57-10-3 | DTXSID2021602

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  - PRODUCT & USE CATEGORIES
  - CHEMICAL WEIGHT FRACTION
  - CHEMICAL FUNCTIONAL USE
  - TOXICS RELEASE INVENTORY
  - MONITORING DATA
  - EXPOSURE PREDICTIONS
  - PRODUCTION VOLUME
- BIOACTIVITY
- SIMILAR COMPOUNDS
- GENRA (BETA)
- RELATED SUBSTANCES
- SYNONYMS
- LITERATURE

Product and Use Categories (PUCs)

Download

Columns | 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

United States Environmental Protection Agency

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Hexadecanoic acid

57-10-3 | DTXSID2021602

Searched by DSSTox Substance Id.

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- GENRA (BETA)
- RELATED SUBSTANCES
- SYNONYMS
- LITERATURE

Chemical Weight Fractions

Download

Columns | 10 | Search query

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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- BIOACTIVITY
- SIMILAR COMPOUNDS
- GENRA (BETA)
- RELATED SUBSTANCES
- SYNONYMS
- LITERATURE
- LINKS
- COMMENTS

Collected Data on Functional Use

Download

Columns

Search query

Harmonized functional use	Reported functional use
fragrance	COLORANT
fragrance	EMOLLIENT
-	emulsifier
fragrance	EMULSIFYING
fragrance	flavorant
fragrance	fragrance
fragrance	Lubricant
-	processing aid
fragrance	Surfactant
fragrance	Surfactants

Predicted Probability of Associated Functional Use
QSAR Version/Date: 2015-11-06

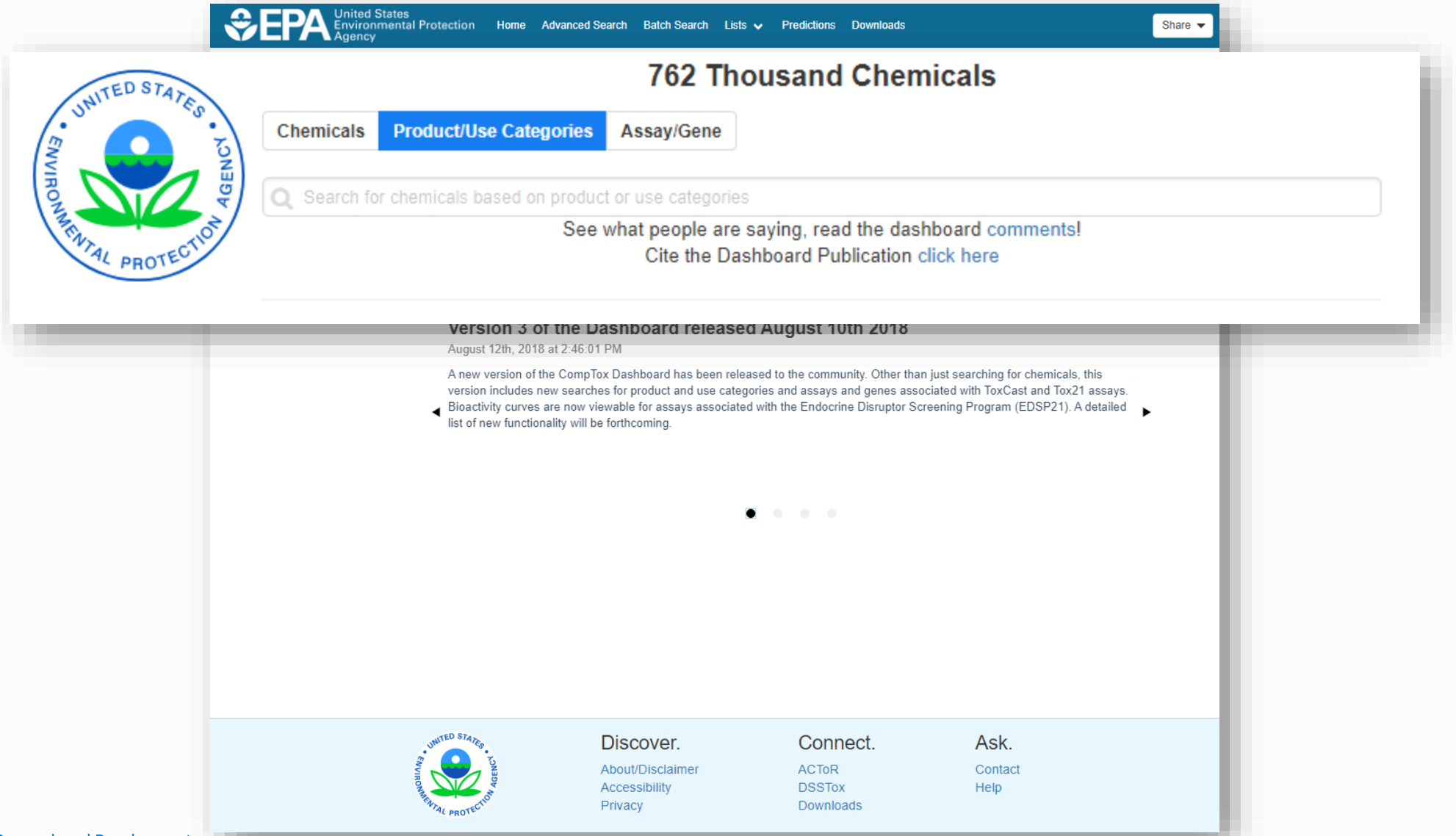
Download

Columns | 10

Search query

Harmonized functional use	Probability
surfactant	0.934
emulsion stabilizer	0.925
lubricating agent	0.951

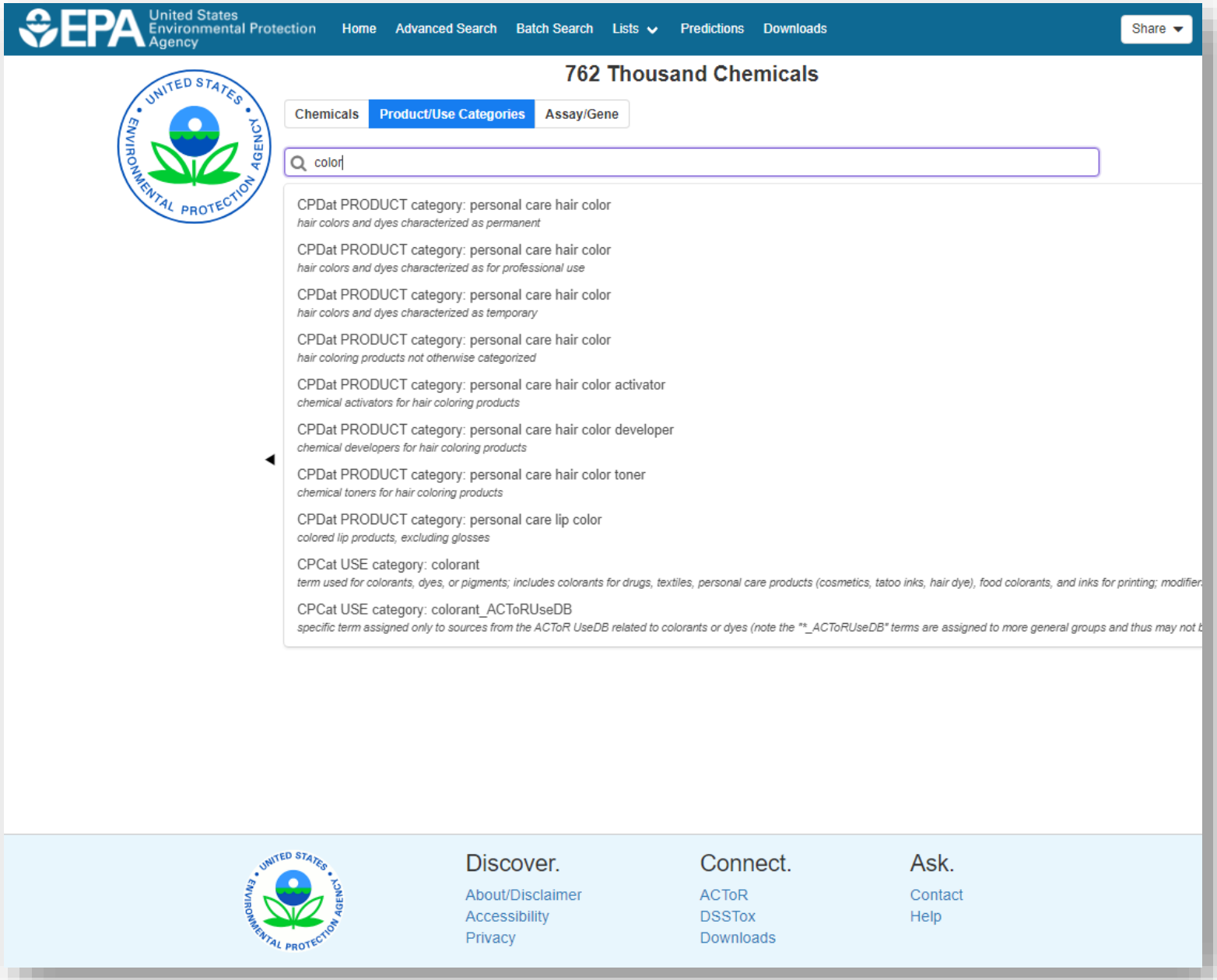
Searching by product and use categories



United States Environmental Protection Agency

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-,...
DTXSID: DTXSID00105105
CASRN: 79873-34-0
TOXCAST: 0

0 related chemical structures with this substance
Lignin, alkali, reaction products with dis...
DTXSID: DTXSID00105862
CASRN: 105859-97-0
TOXCAST: 0

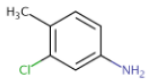
0 related chemical structures with this substance
Octadecanoic acid, 12-hydroxy-, homop...
DTXSID: DTXSID00106172
CASRN: 124578-12-7
TOXCAST: 0

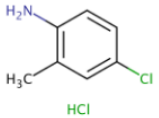
0 related chemical structures with this substance
Naphthalenesulfonic acid, methyl-, poly...
DTXSID: DTXSID00108419
CASRN: 81065-51-2
TOXCAST: 0

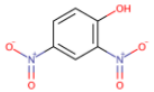
0 related chemical structures with this substance
C.I. Direct Blue 42
DTXSID: DTXSID00108772
CASRN: 6426-71-7
TOXCAST: 0

0 related chemical structures with this substance
C.I. Direct Brown 13
DTXSID: DTXSID00108777
CASRN: 8003-82-5
TOXCAST: 0

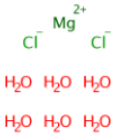
0 related chemical structures with this substance
Poly(oxy-1,2-ethanediyl), alpha-tridecyl-...
DTXSID: DTXSID00110077
CASRN: 69011-36-5
TOXCAST: 0


3-Chloro-4-methylaniline
DTXSID: DTXSID0020286
CASRN: 95-74-9
TOXCAST: 5/297


4-Chloro-2-methylaniline hydrochloride
DTXSID: DTXSID0020288
CASRN: 3165-93-3
TOXCAST: 9/276

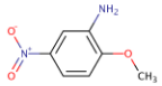

2,4-Dinitrophenol
DTXSID: DTXSID0020523
CASRN: 51-28-5
TOXCAST: 32/508

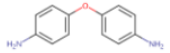
Ethylene oxide
DTXSID: DTXSID0020600
CASRN: 75-21-8
TOXCAST: 0


Magnesium chloride hexahydrate
DTXSID: DTXSID0020789
CASRN: 7791-18-6
TOXCAST: 3/113

Dichloromethane
DTXSID: DTXSID0020868
CASRN: 75-09-2
TOXCAST: 1/113

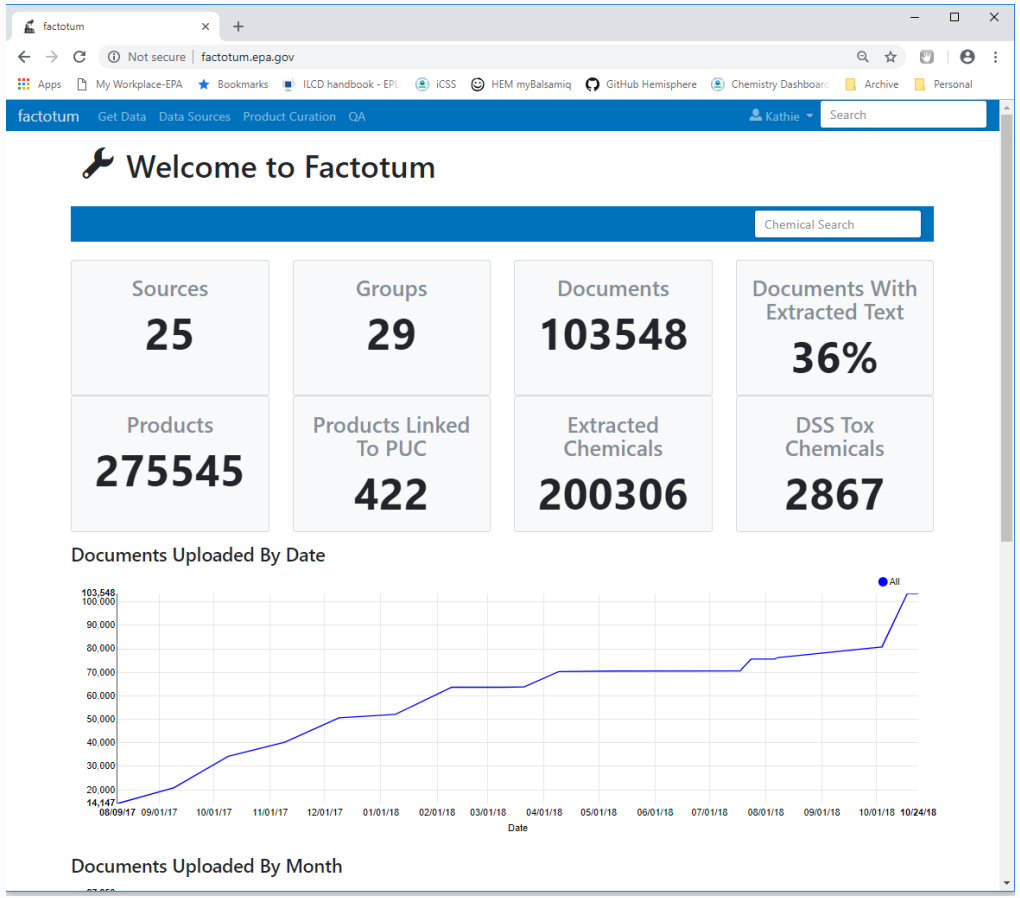
Sodium nitrite
DTXSID: DTXSID0020941
CASRN: 7632-00-0
TOXCAST: 3/537

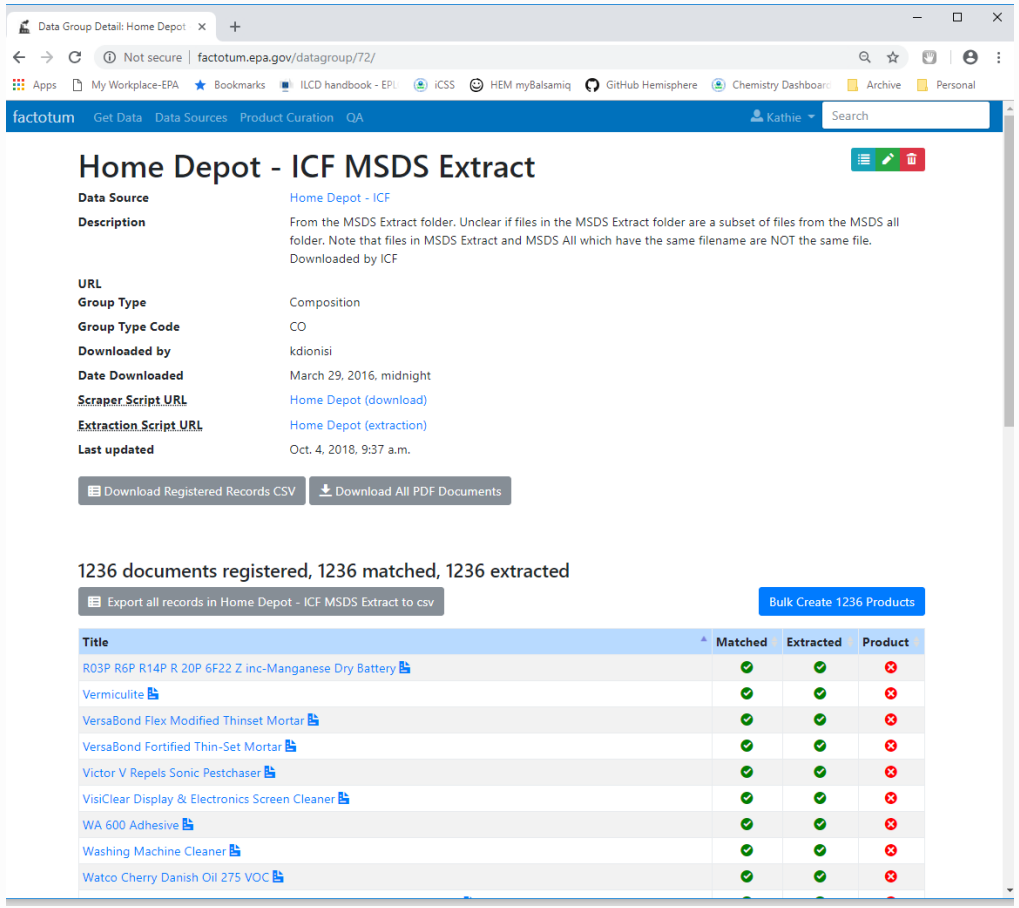

2-Methoxy-5-nitroaniline
DTXSID: DTXSID0020943
CASRN: 99-59-2
TOXCAST: 14/572


4,4'-Oxydianiline
DTXSID: DTXSID0021094
CASRN: 101-80-4
TOXCAST: 29/589

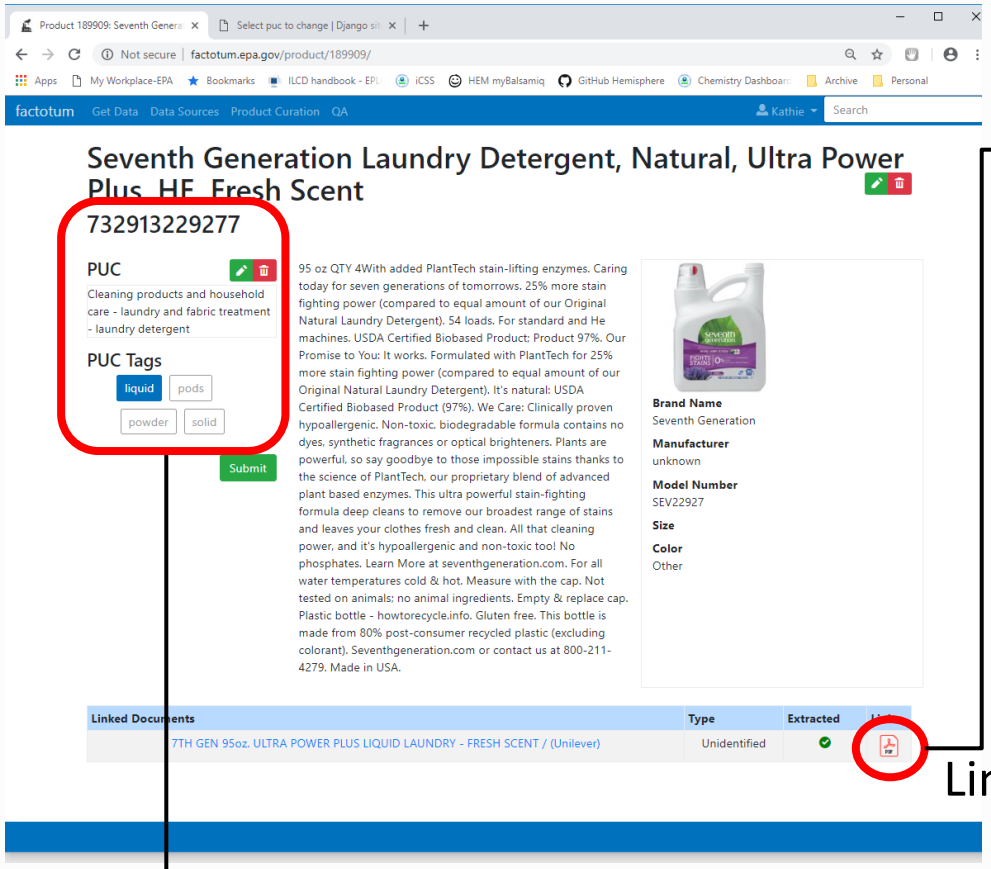
1 related chemical structure with this substance
Polysorbate 80
DTXSID: DTXSID0021175
CASRN: 9005-65-6
TOXCAST: 10/297

Internal data management

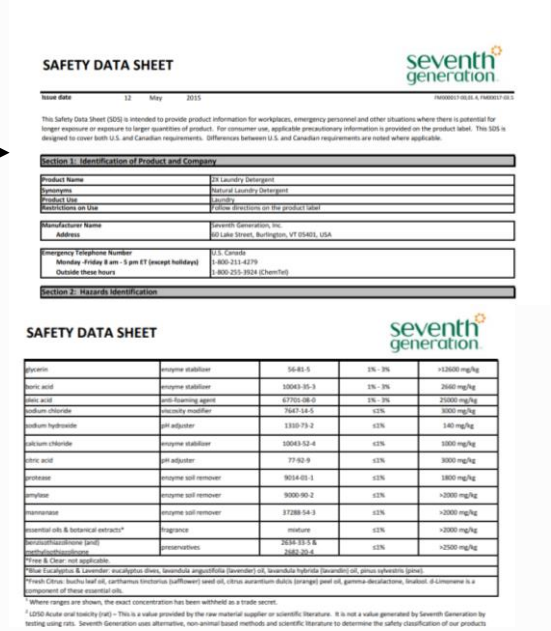




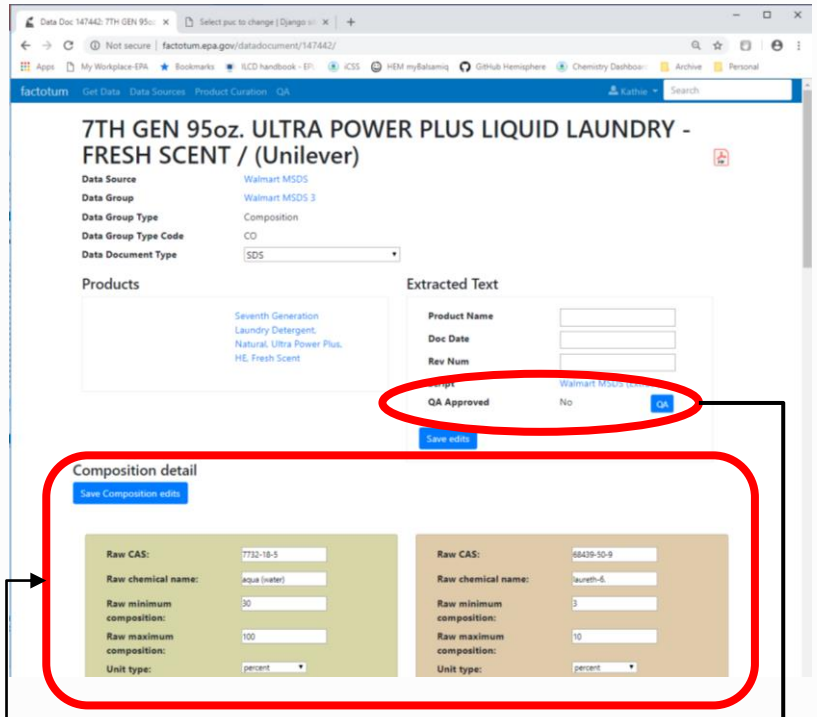
Internal data management



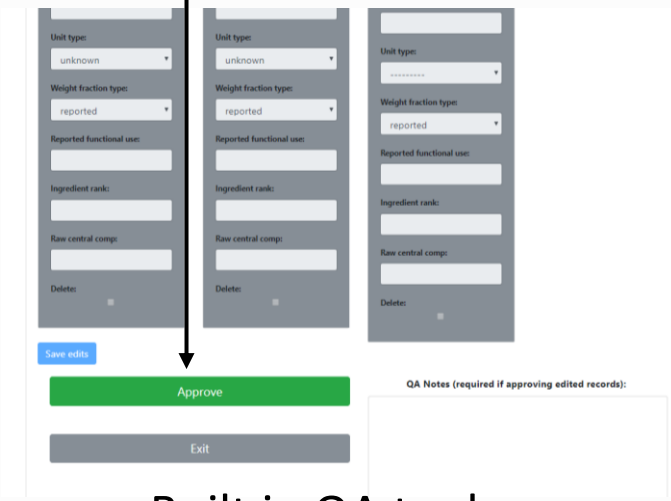
Product UPC & Product category (PUC) assignment



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
Richard Judson
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John Wambaugh (RED)
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EPA - NERL
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Kristin Isaacs (RED)
Abhishek Komandur*
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

Special thanks to coauthors Kristin Isaacs and Katherine Phillips for slide material.