https://orcid.org/0000-0001-9547-1654

EPA United States Environmental Protection Agency

Physicians Committee for Responsible Medicine

NURA™

Data and Models from the ExpoCast Project for Informing Chemical Assessment

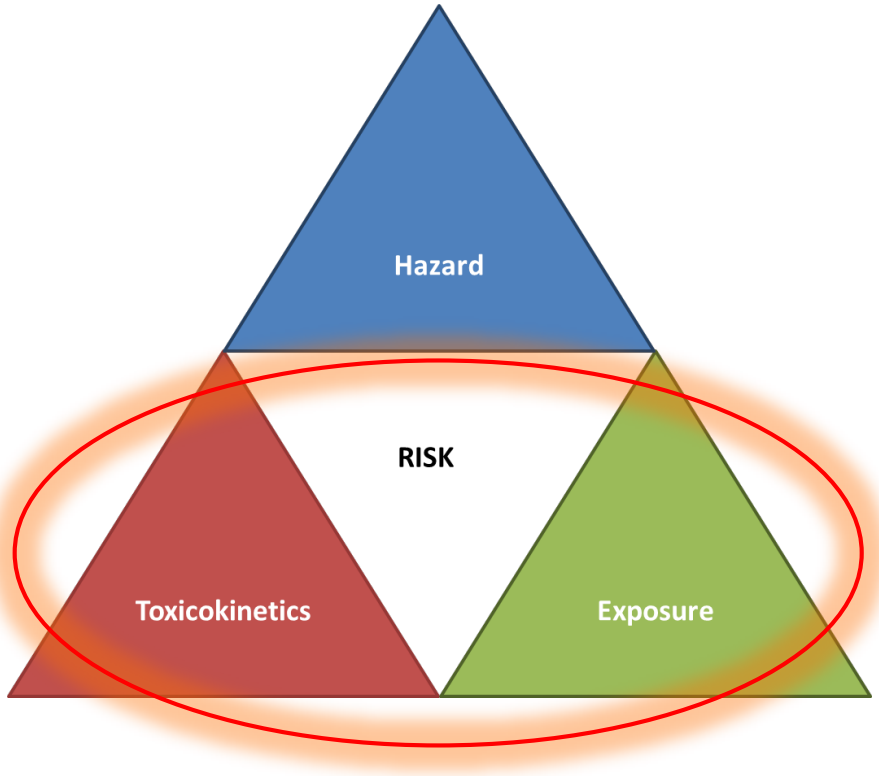
Kristin Isaacs, PhD
Isaacs.kristin@epa.gov

Center for Computational Toxicology and Exposure, US-EPA, RTP, NC

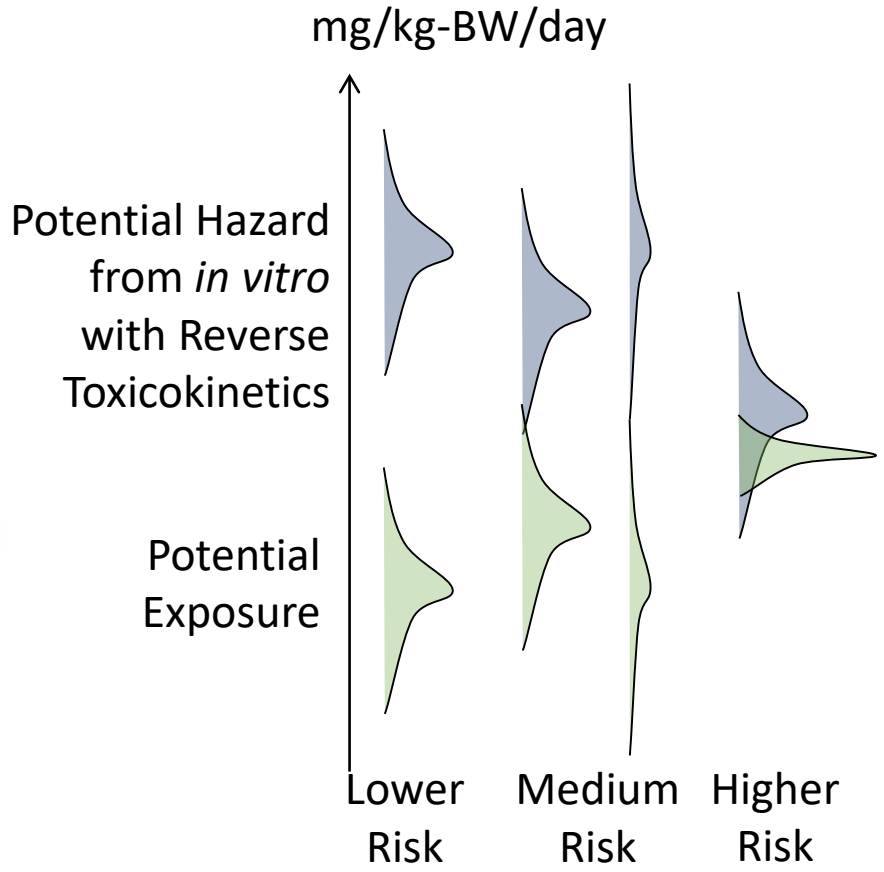
The views expressed in this presentation are those of the authors and do not necessarily reflect the views or policies of the U.S. EPA

10/23/2020
Happy Mole Day!

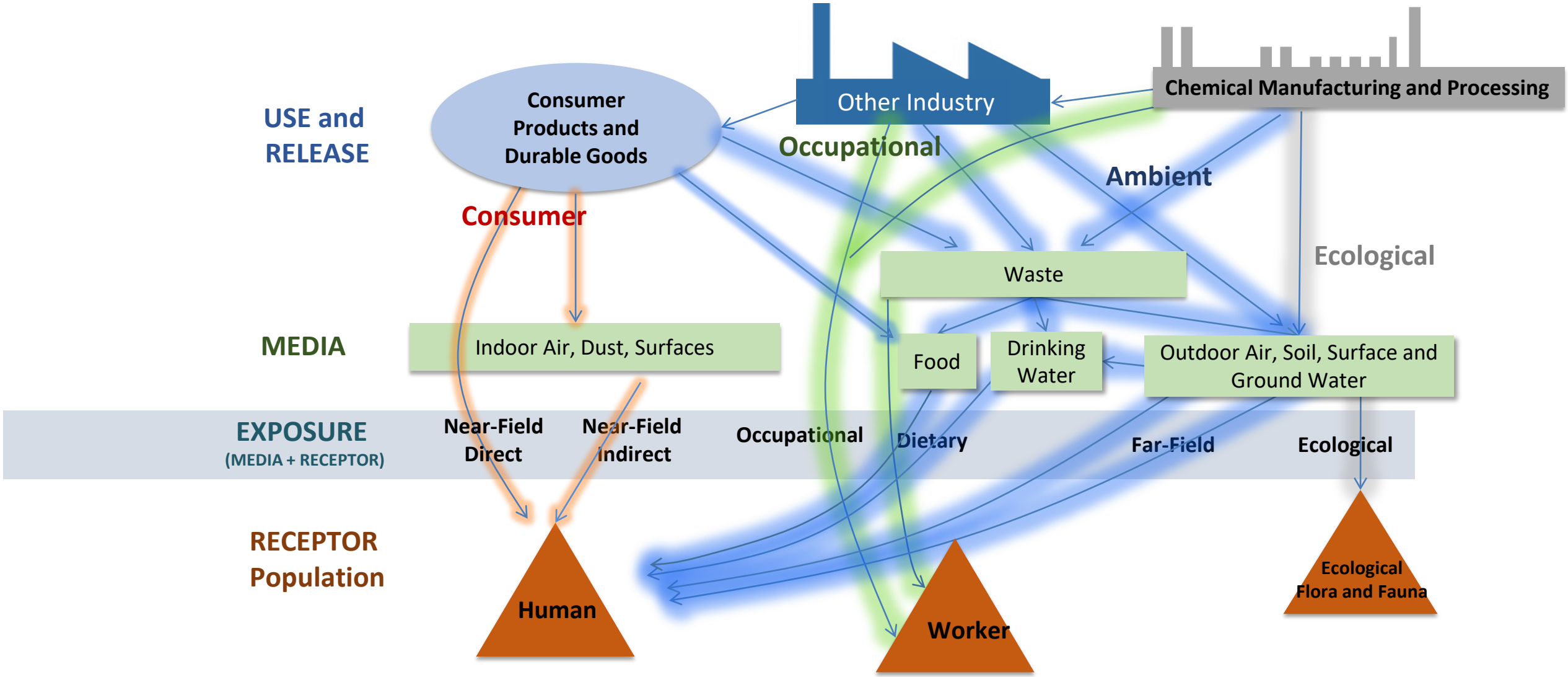
Risk is Multifaceted



EPA's ExpoCast Project

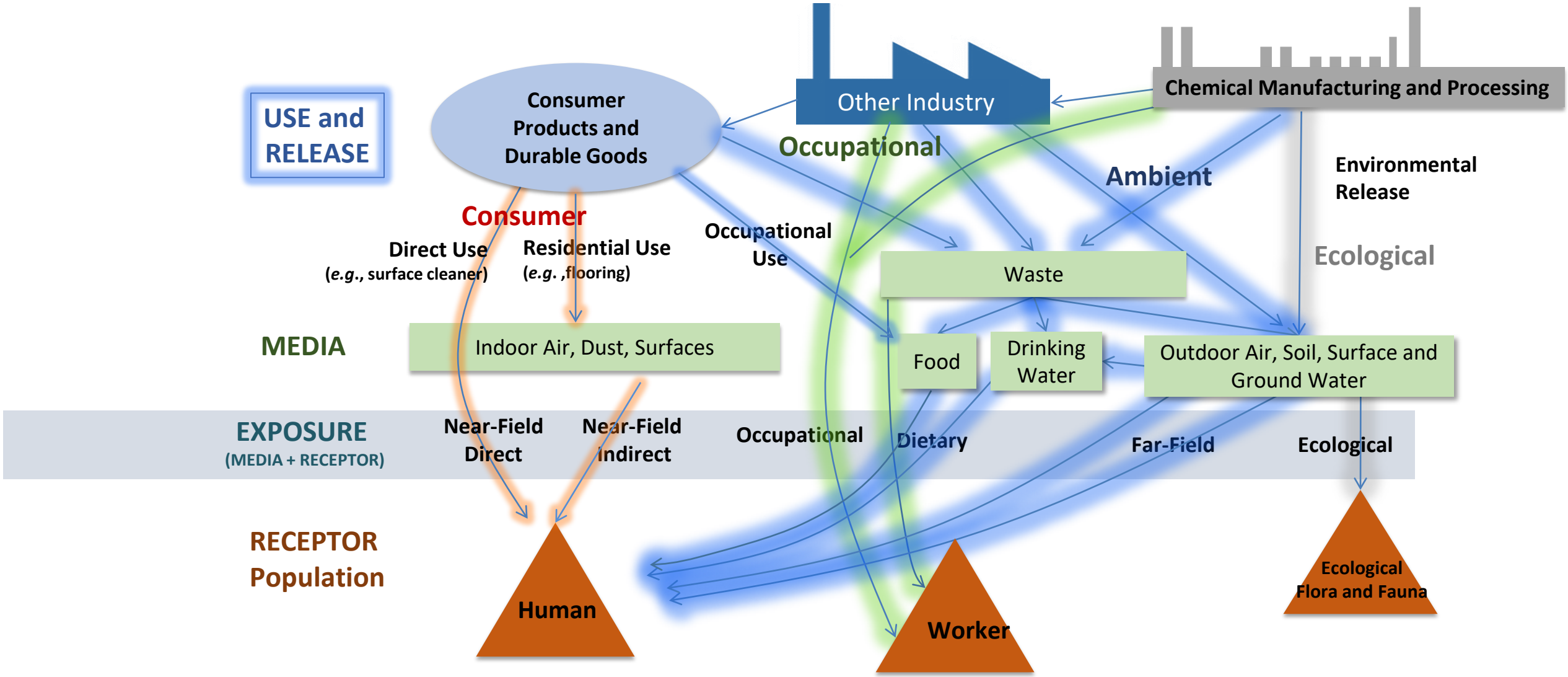


Exposure Pathways



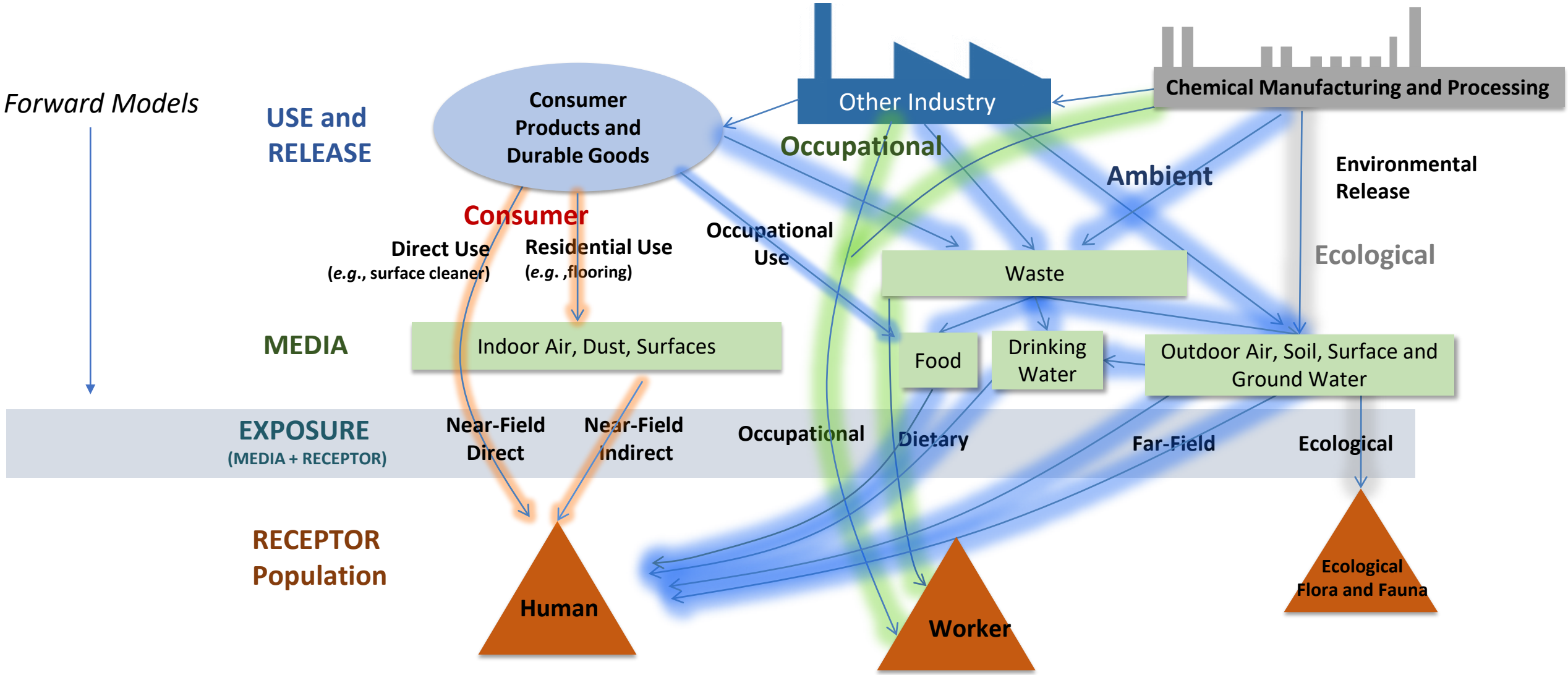
Exposure Pathways

EPA United States Environmental Protection Agency



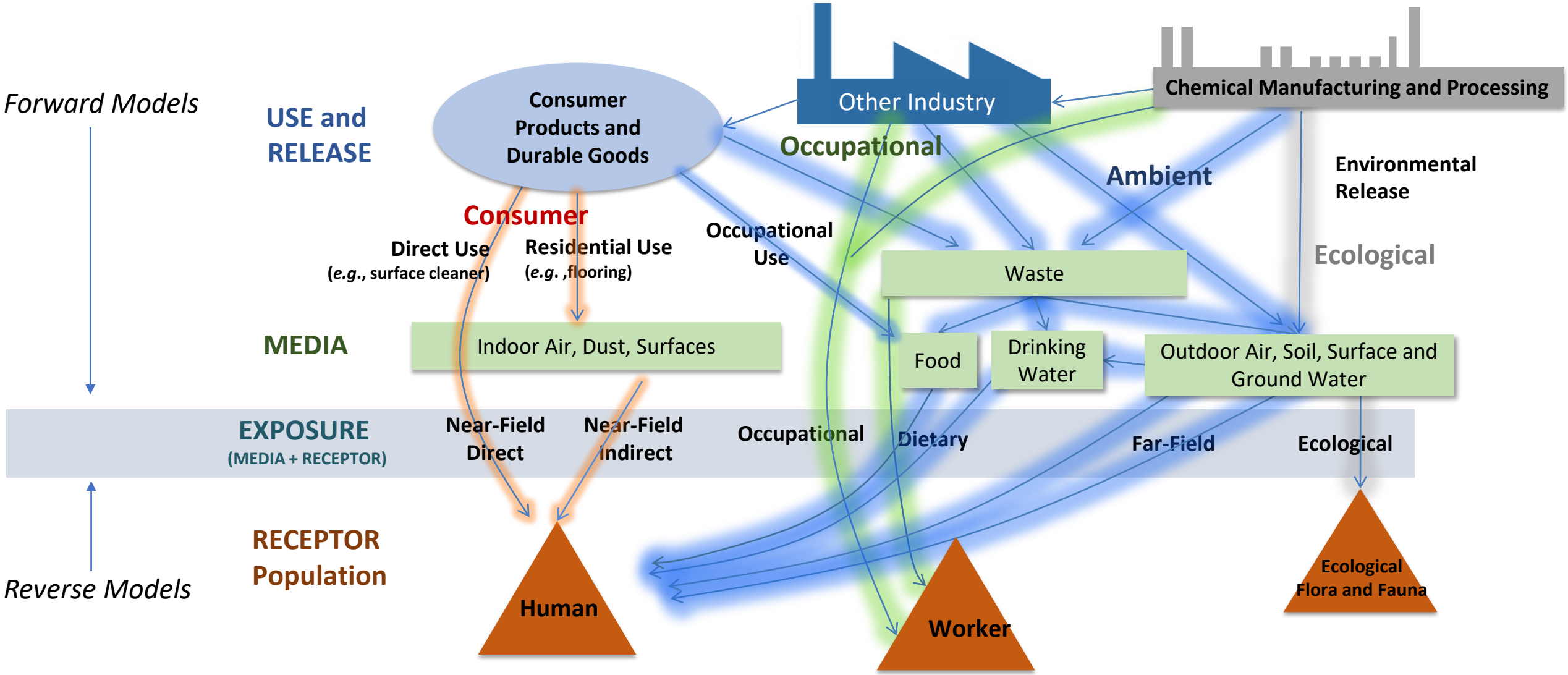
Exposure Pathways

EPA United States Environmental Protection Agency



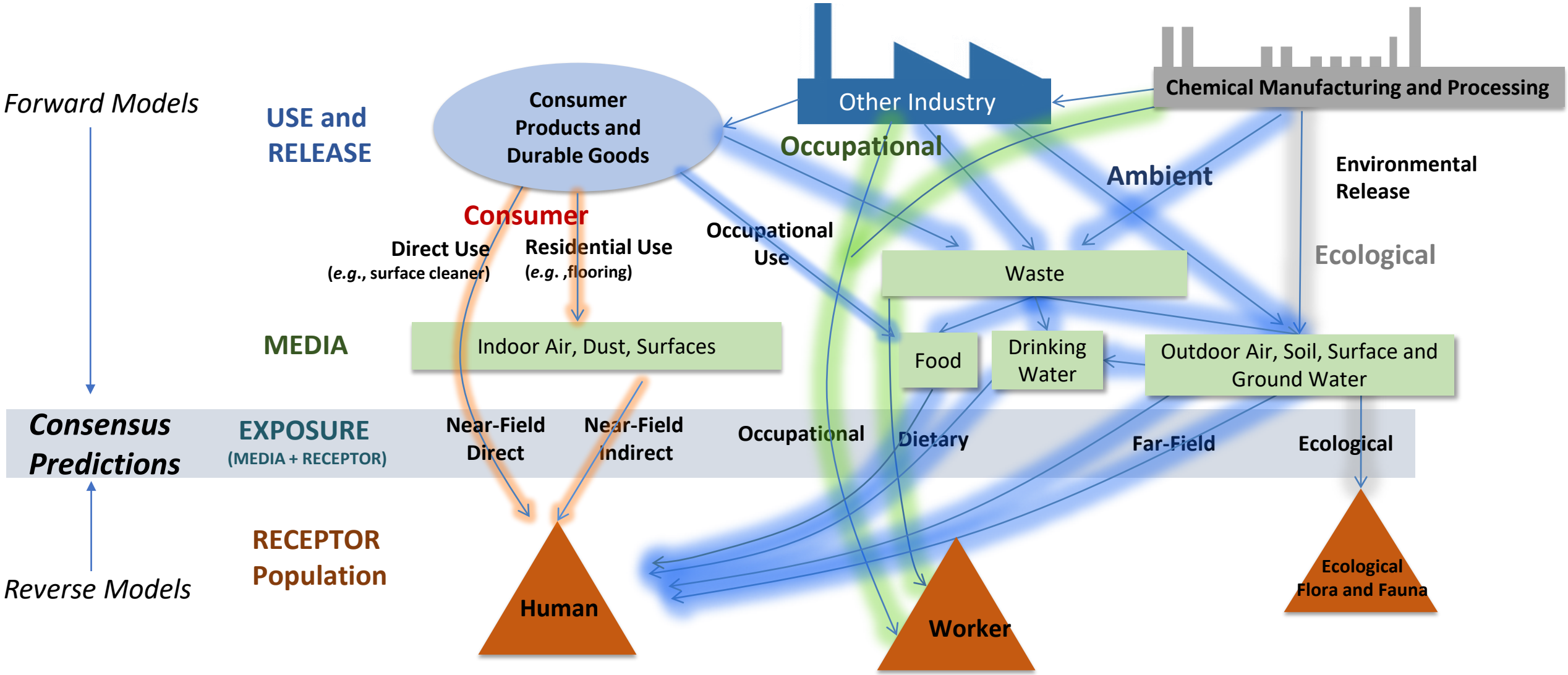
Exposure Pathways

United States Environmental Protection Agency



Exposure Pathways

United States Environmental Protection Agency



The Chemicals and Products Database (CPDat)

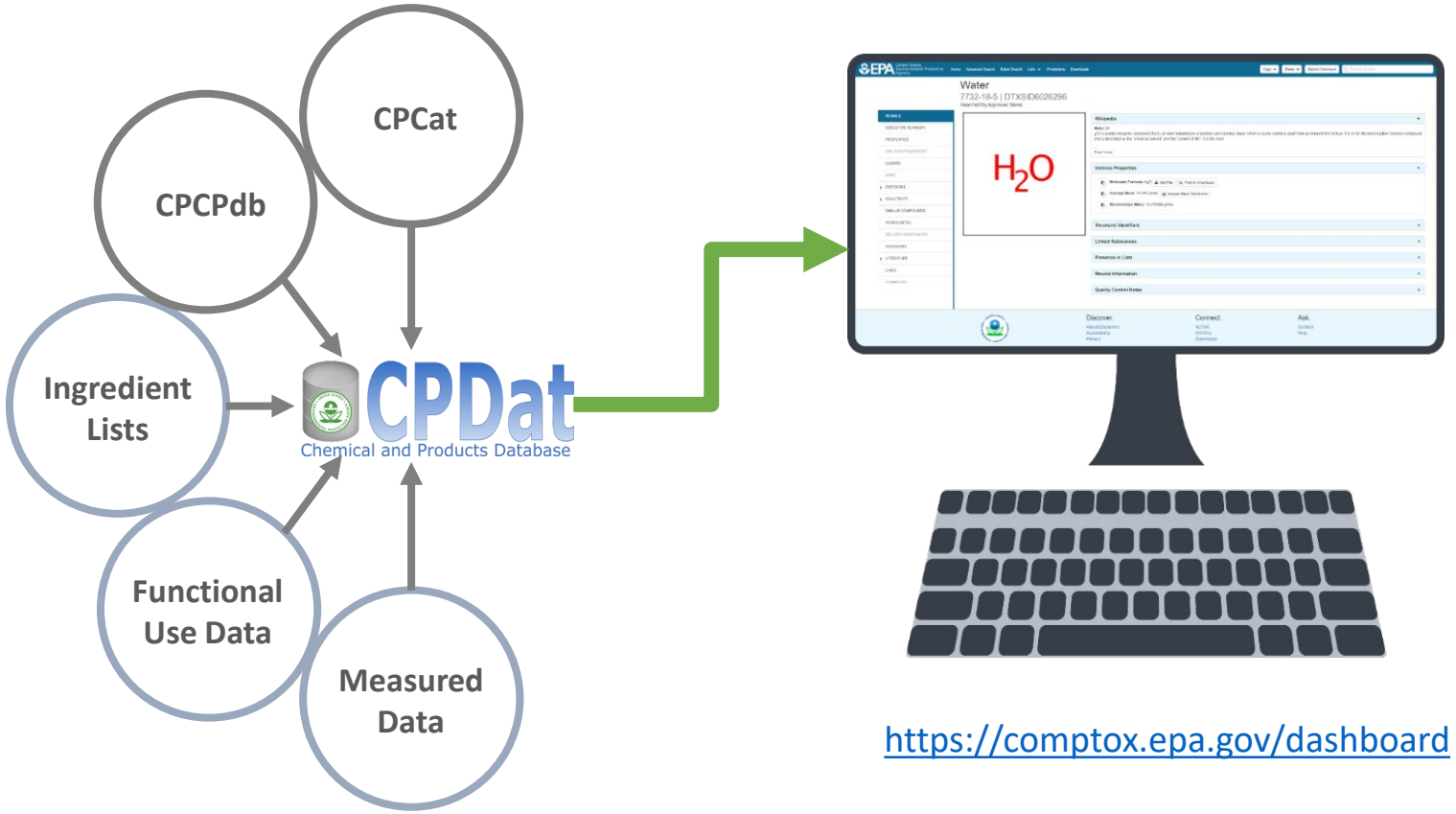
EPA United States Environmental Protection Agency

- 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
- Sustainable way to ***organize, update, and disseminate these data***

CPDat
Chemical and Products Database

CompTox Dashboard

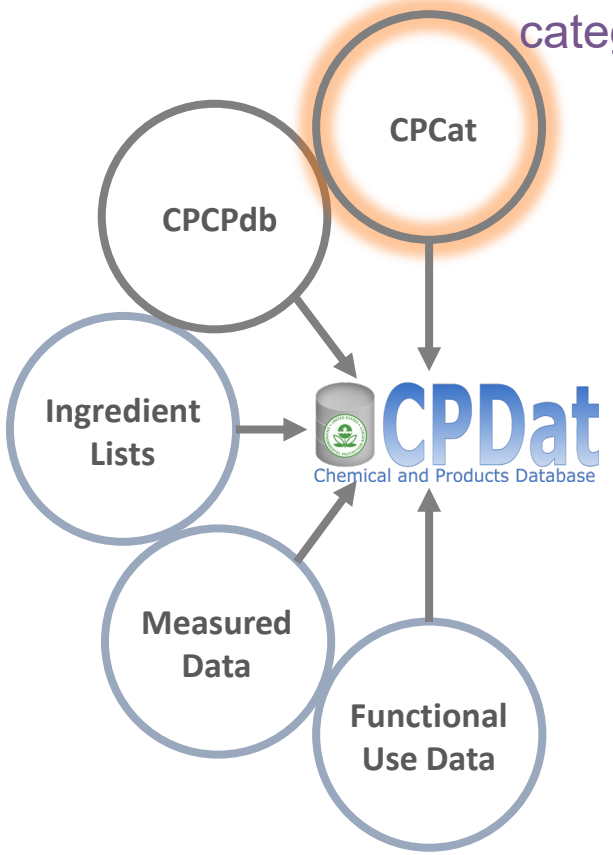
What is CPDat?

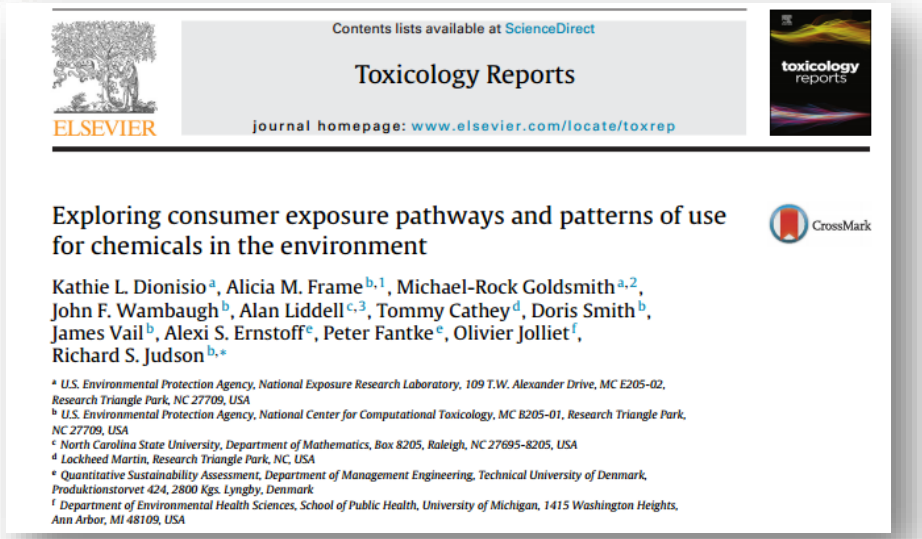


https://comptox.epa.gov/dashboard

What is CPDat?

General use categories





Contents lists available at ScienceDirect

Toxicology Reports

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

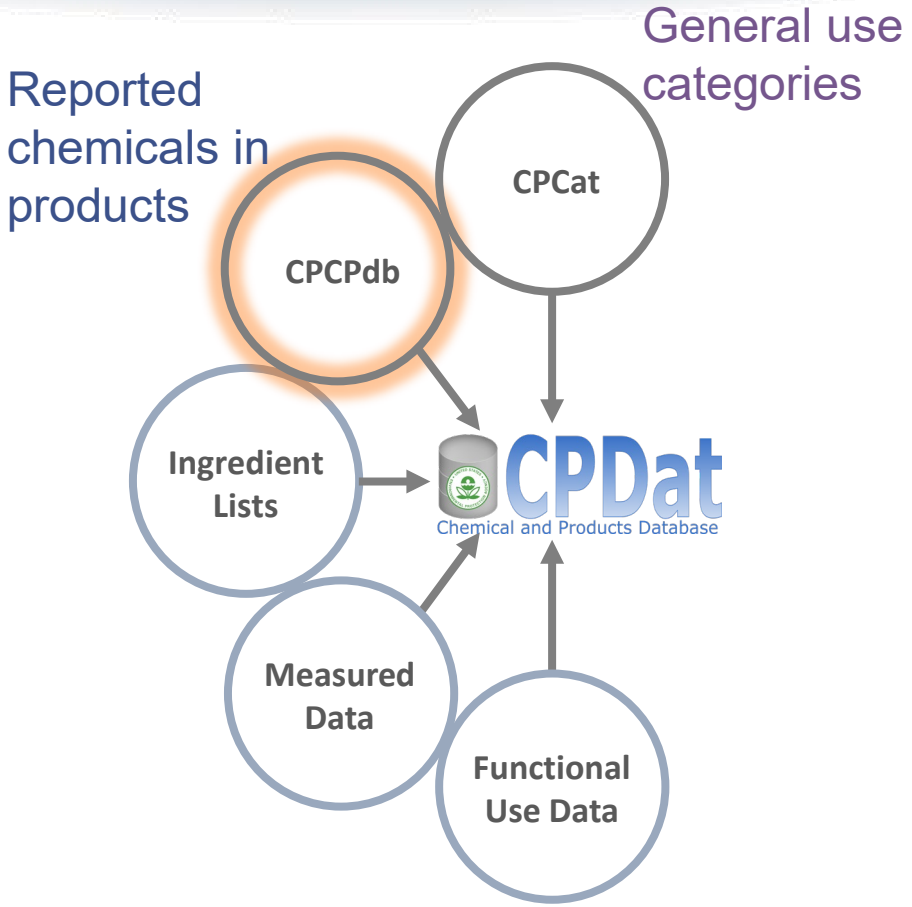
Exploring consumer exposure pathways and patterns of use for chemicals in the environment

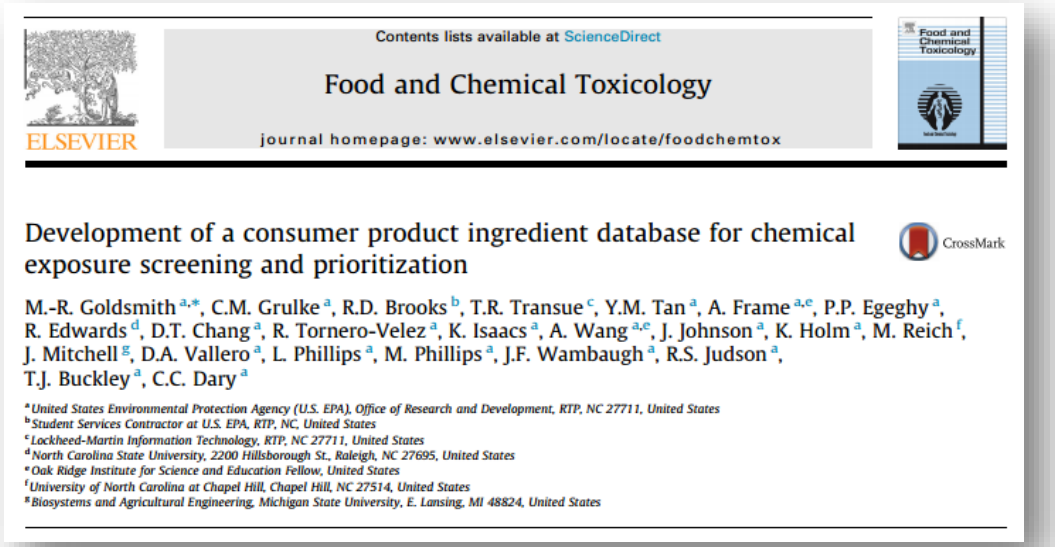
Kathie L. Dionisio[a], Alicia M. Frame[b,1], Michael-Rock Goldsmith[a,2], John F. Wambaugh[b], Alan Liddell[c,3], Tommy Cathey[d], Doris Smith[b], James Vail[b], Alexi S. Ernstoff[e], Peter Fantke[e], Olivier Jolliet[f], Richard S. Judson[b,*]

[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

- Presence on other chemical lists
- Broad categorization of chemical use
  - Therapeutic use
  - Consumer product-based use
  - Industrial process use
- Curated to a large number of relevant index terms

What is CPDat?





Contents lists available at ScienceDirect

Food and Chemical Toxicology

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

ELSEVIER

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

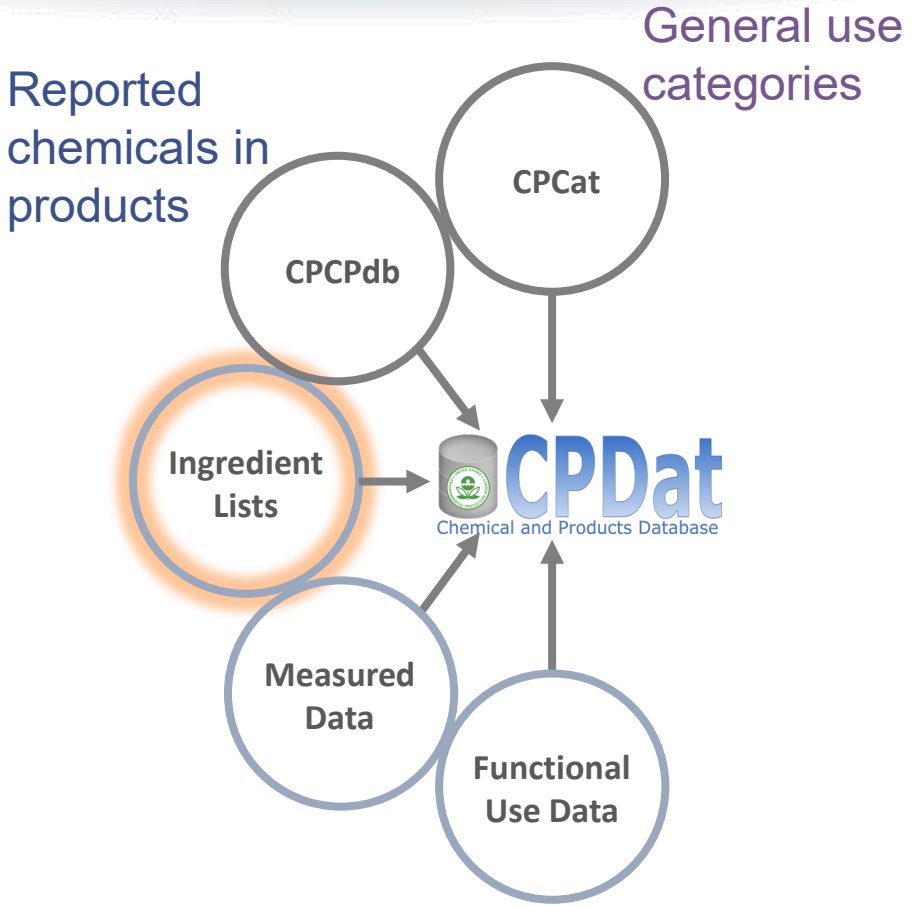
CrossMark

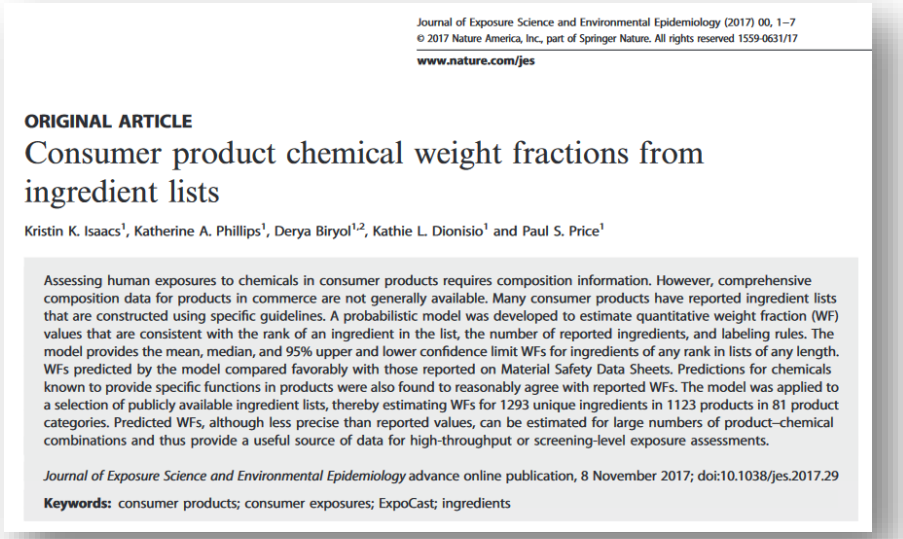
M.-R. Goldsmith [a,*], C.M. Grulke [a], R.D. Brooks [b], T.R. Transue [c], Y.M. Tan [a], A. Frame [a,e], P.P. Egeghy [a], R. Edwards [d], D.T. Chang [a], R. Tornero-Velez [a], K. Isaacs [a], A. Wang [a,e], J. Johnson [a], K. Holm [a], M. Reich [f], J. Mitchell [g], D.A. Vallero [a], L. Phillips [a], 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
© 2017 Nature America, Inc., part of Springer Nature. All rights reserved 1559-0631/17
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]

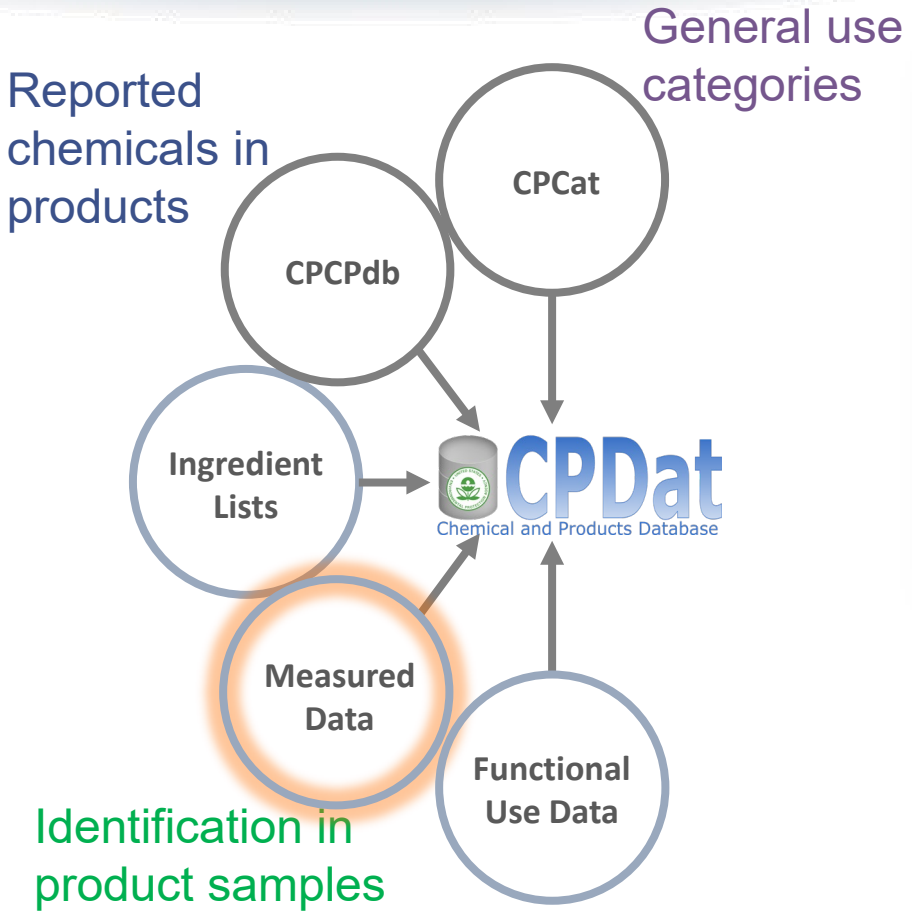
Assessing human exposures to chemicals in consumer products requires composition information. However, comprehensive composition data for products in commerce are not generally available. Many consumer products have reported ingredient lists that are constructed using specific guidelines. A probabilistic 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.

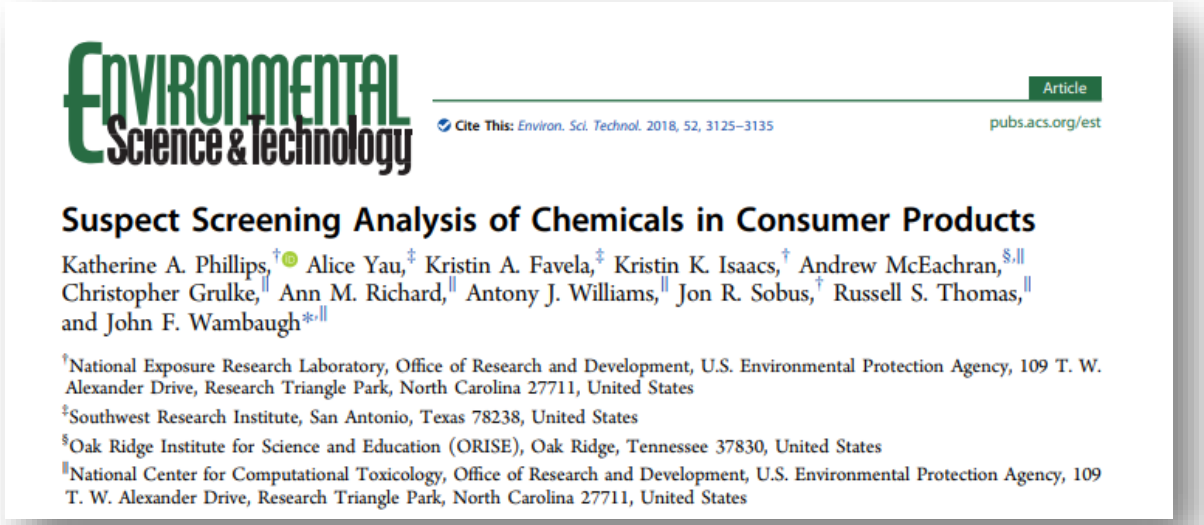
Journal of Exposure Science and Environmental Epidemiology advance online publication, 8 November 2017; doi:10.1038/jes.2017.29

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?





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

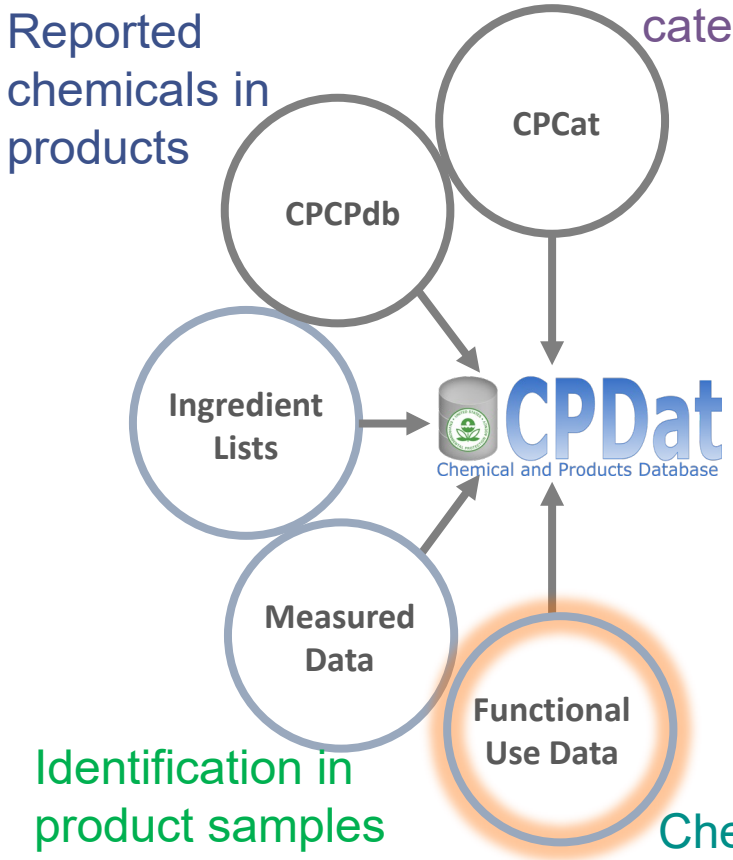
[‡]Southwest Research Institute, San Antonio, Texas 78238, United States

[§]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?



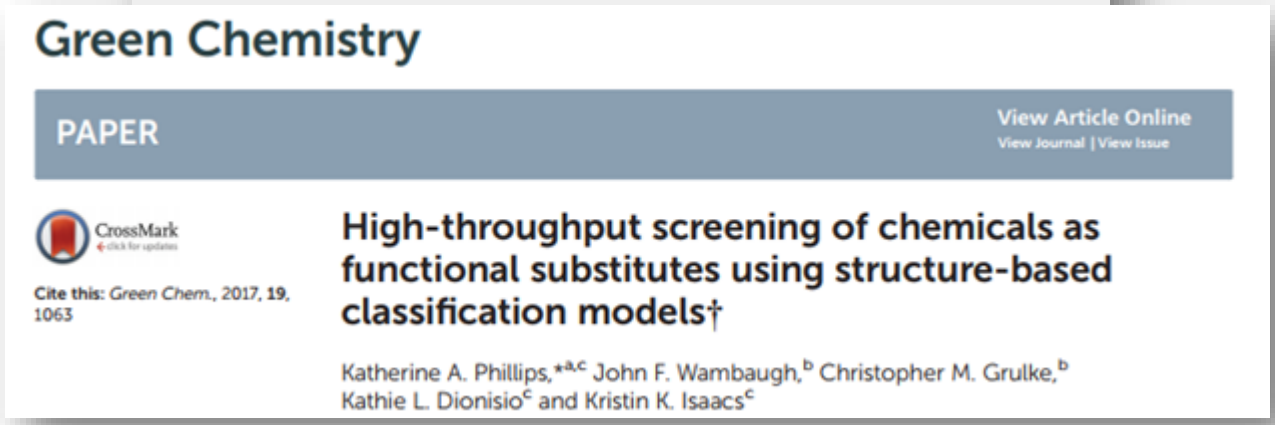

Contents lists available at ScienceDirect

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]


Green Chemistry

PAPER

View Article Online
View Journal | View Issue

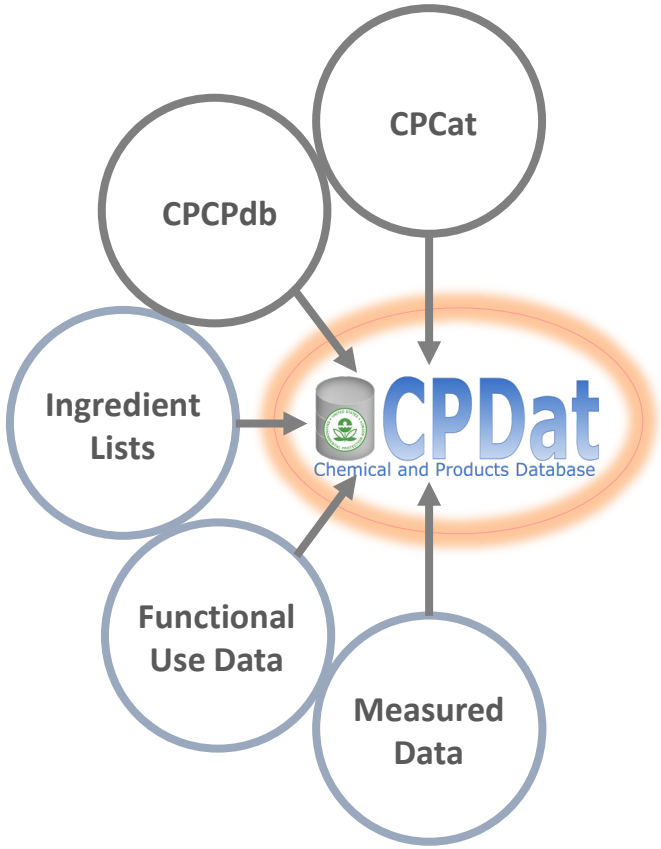
Cite this: Green Chem., 2017, 19, 1063

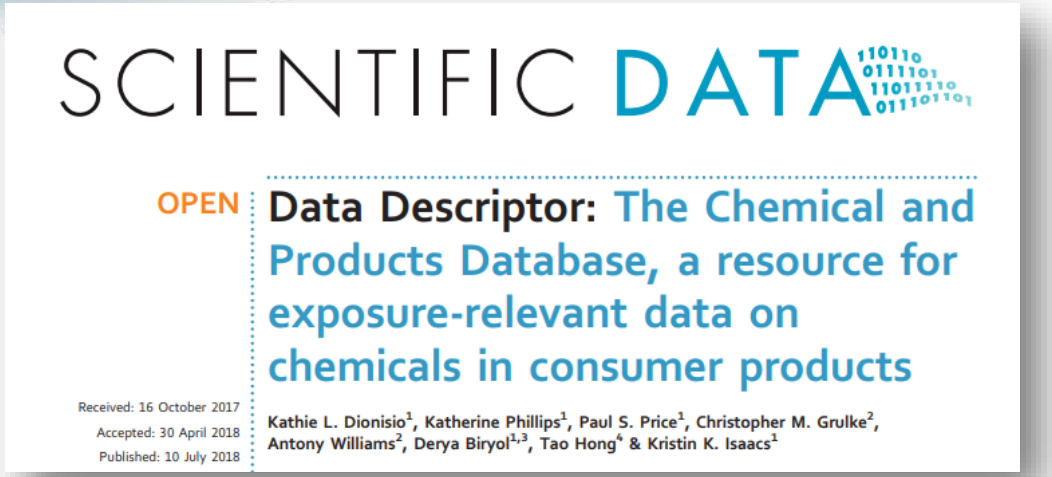
High-throughput screening of chemicals as functional substitutes using structure-based classification models†

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
  - Function Predictions

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

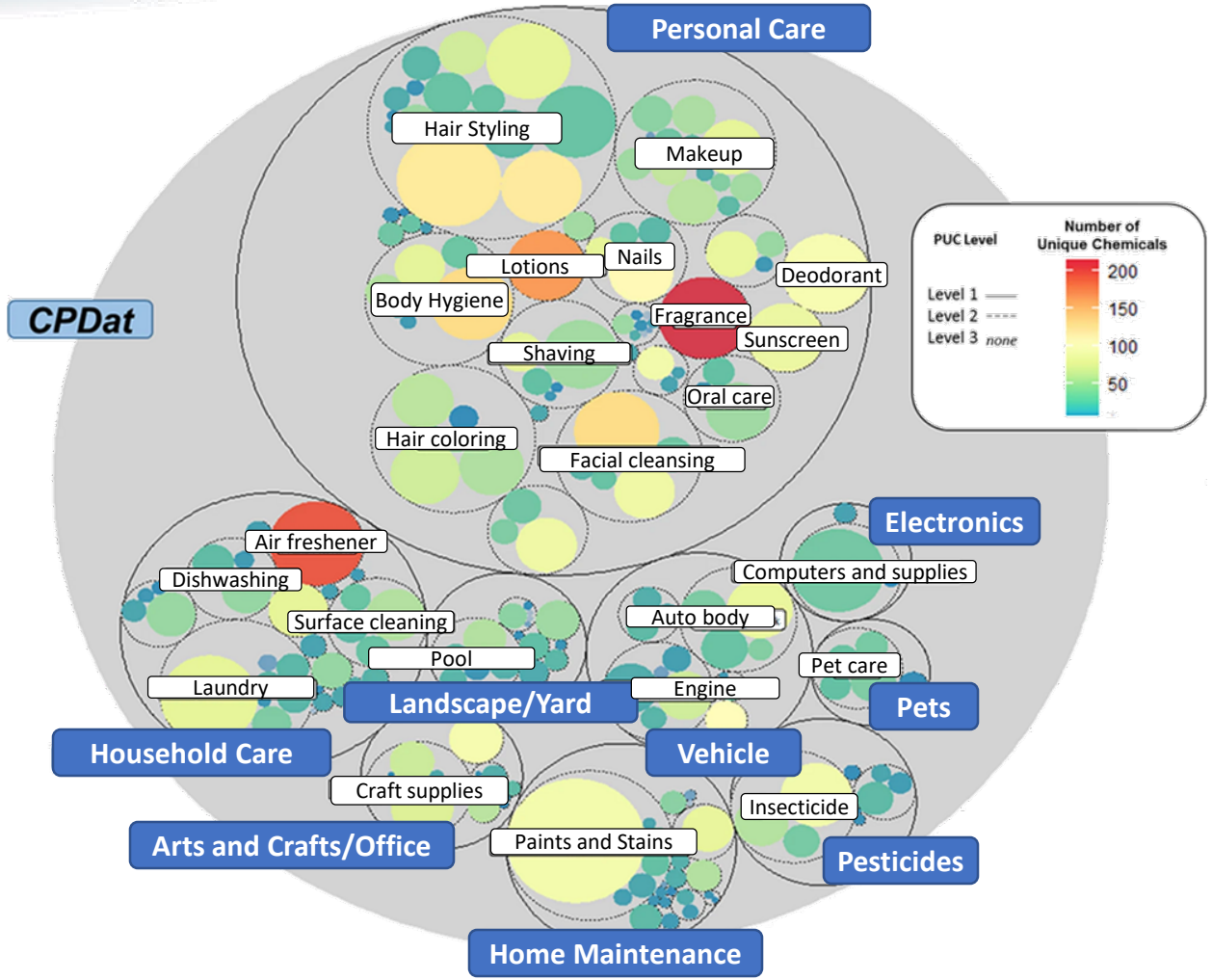
Kathie L. Dionisio[1], Katherine Phillips[1], Paul S. Price[1], Christopher M. Grulke[2], Antony Williams[2], Derya Biryol[1,3], Tao Hong[4] & Kristin K. Isaacs[1]

- 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

Product Categories in CPDat

United States Environmental Protection Agency

- Allows for linking to consumer product exposure models
  - Maps to habits and practices (product use) data
  - Maps to exposure algorithms – if chemical and product are known, models can be rapidly parameterized

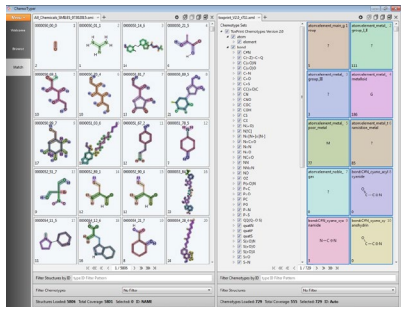


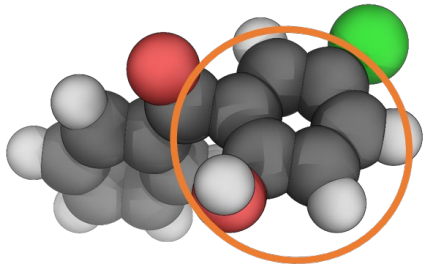
Isaacs et al., 2019

Predictive Models for Chemical Function

United States Environmental Protection Agency

Chemical Structure and Property Descriptors





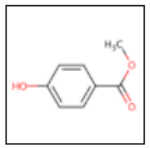
Chemical Function Information (CPDat Reported)

Machine-Learning Based Classification Models

Prediction of Of Potential Functions for Unclassified Chemicals (**Available in CPDat**)

Phillips et al., 2017

CPDat Data in the Dashboard

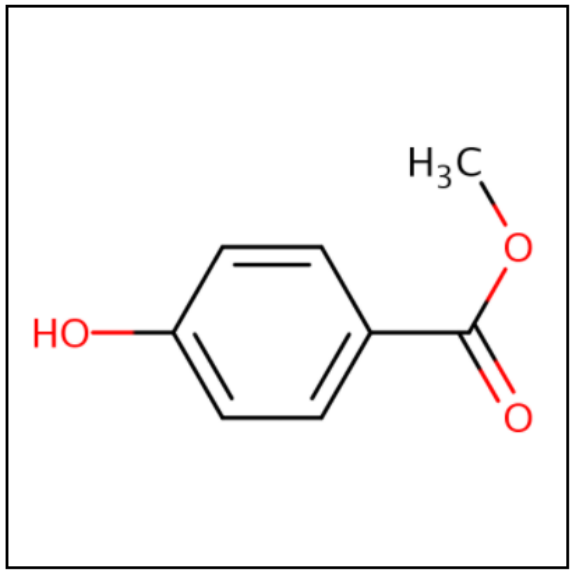


Methylparaben

99-76-3 | DTXSID4022529

Searched by Synonym from Valid Source.

- DETAILS
- EXECUTIVE SUMMARY
- PROPERTIES
- ENV. FATE/TRANSPORT
- HAZARD
- SAFETY
- ADME
- EXPOSURE
- BIOACTIVITY
- SIMILAR COMPOUNDS
- GENRA (BETA)
- RELATED SUBSTANCES
- SYNONYMS
- LITERATURE
- LINKS
- COMMENTS



Wikipedia

Methylparaben, also **methyl paraben**, one of the parabens, is a preservative with the chemical formula $CH_3(C_6H_4(OH)COO)$. It is the methyl ester of *p*-hydroxybenzoic acid.

...

Read more

Quality Control Notes

Intrinsic Properties

Molecular Formula: $C_8H_8O_3$ | Mol File | Find All Chemicals

Average Mass: 152.149 g/mol | Isotope Mass Distribution

Monoisotopic Mass: 152.047344 g/mol

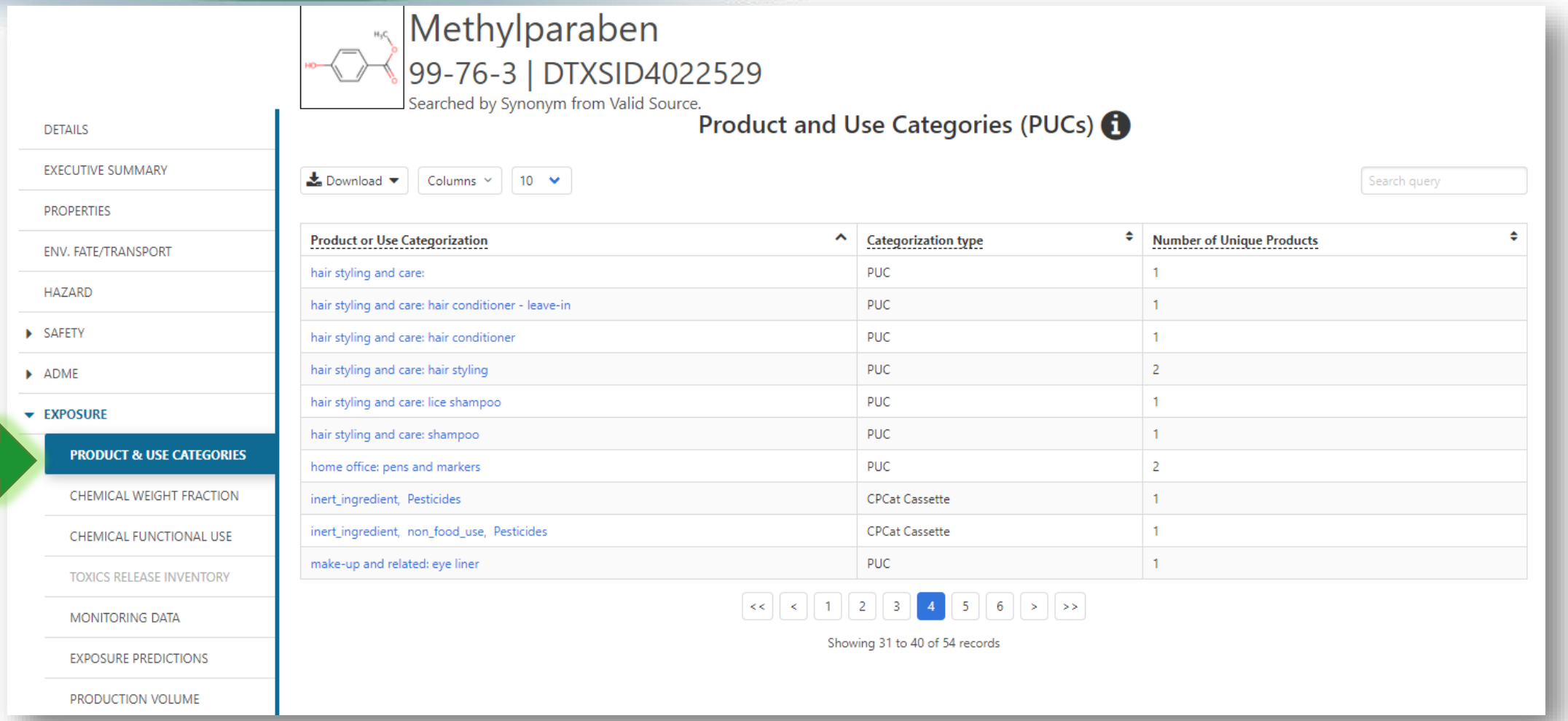
Structural Identifiers

Linked Substances

Presence in Lists

Record Information

CPDat Data in the Dashboard



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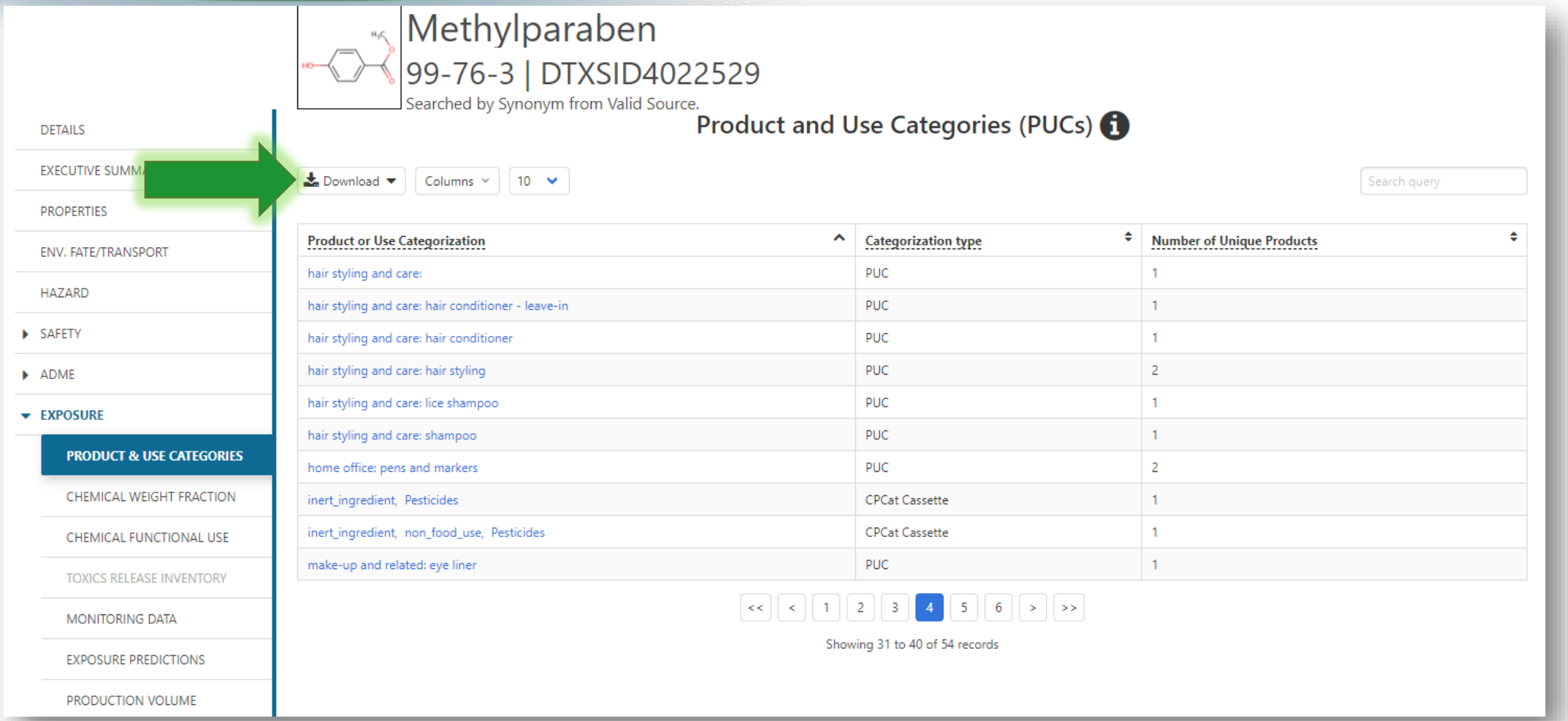
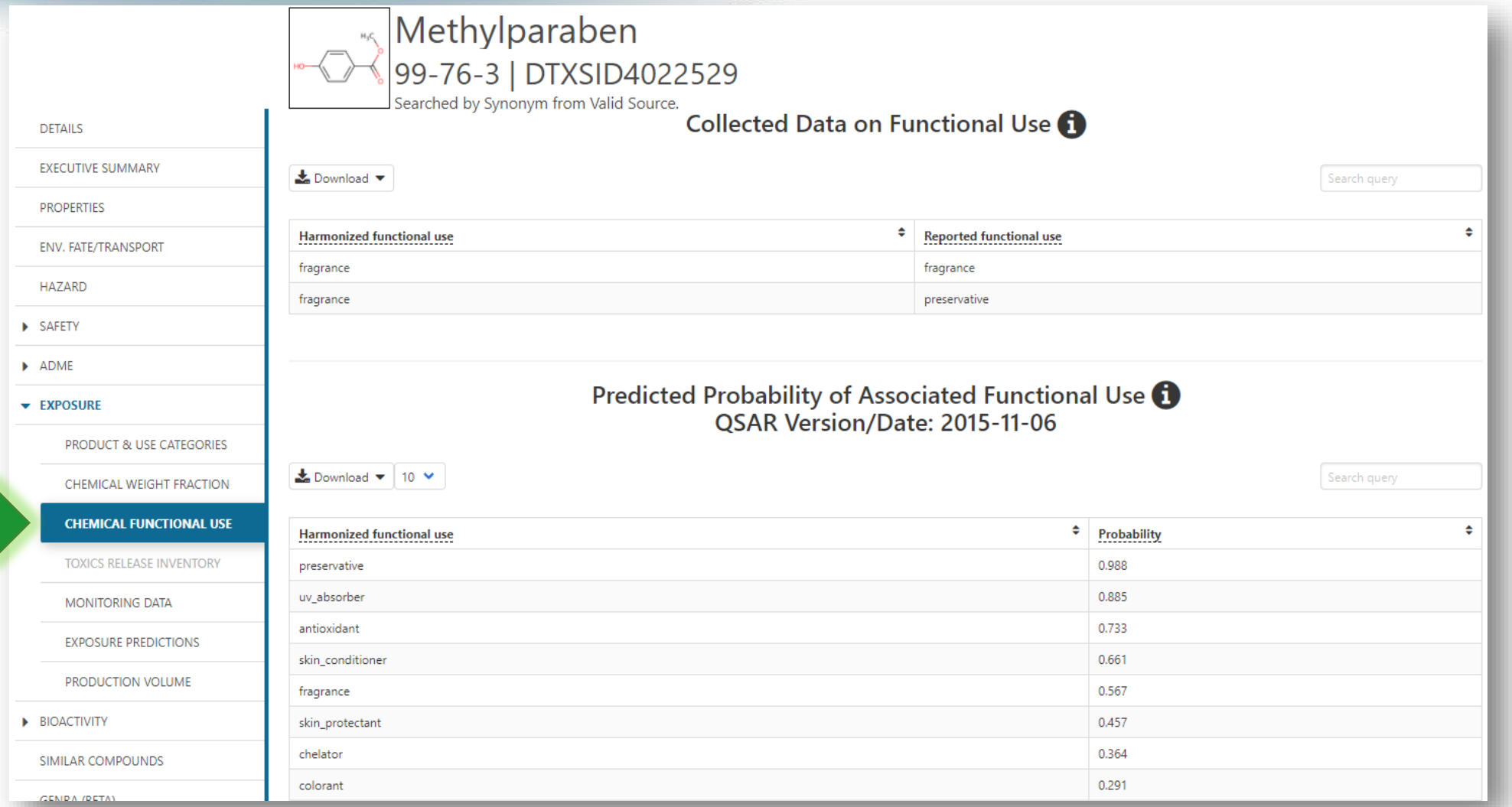


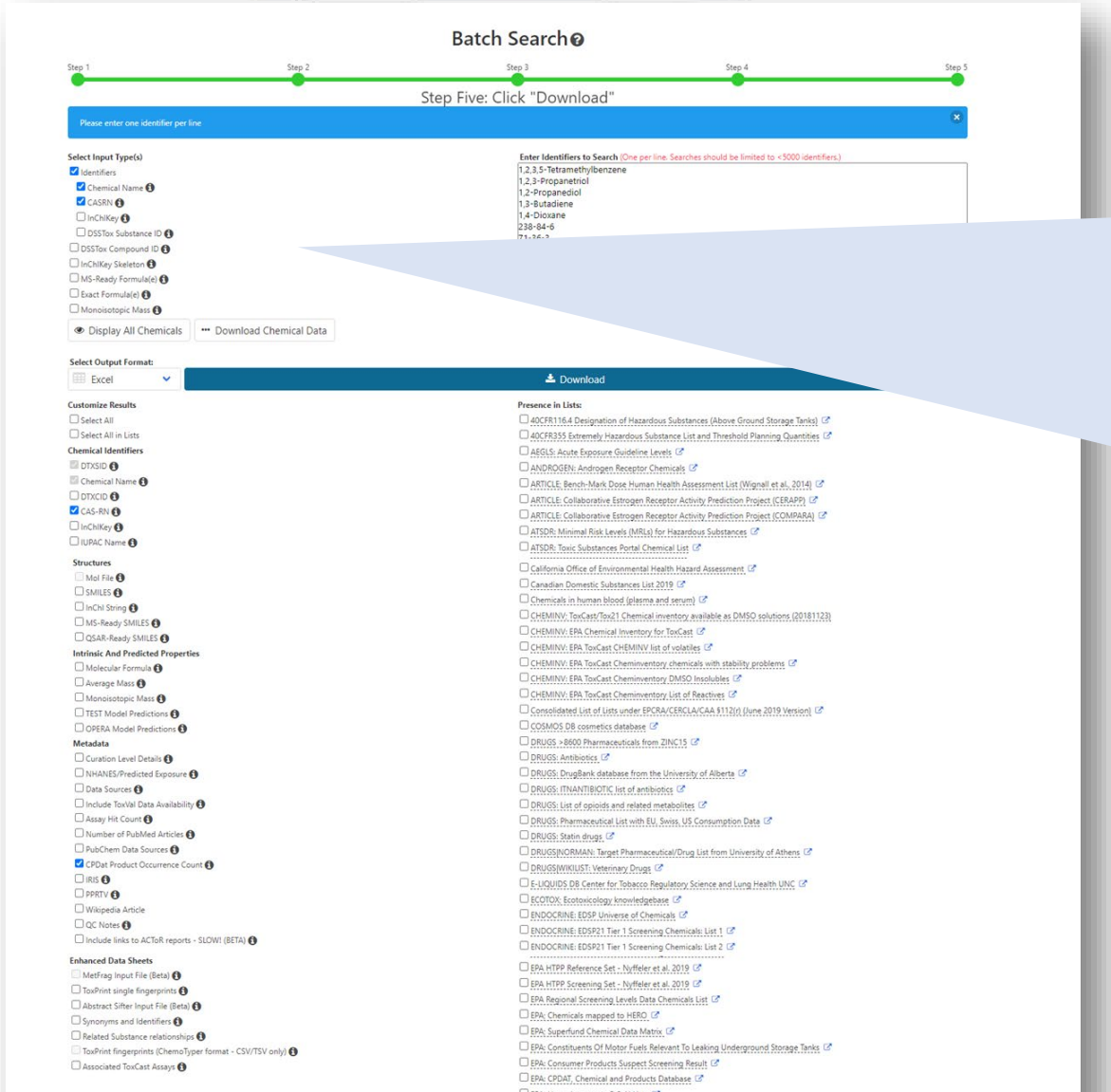
All category data for a chemical can be downloaded

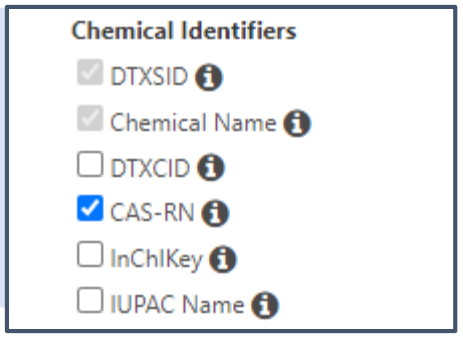
CPDat Data in the Dashboard



CPDat Data in the Dashboard

United States Environmental Protection Agency





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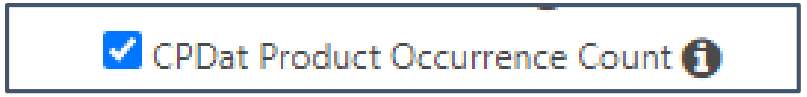

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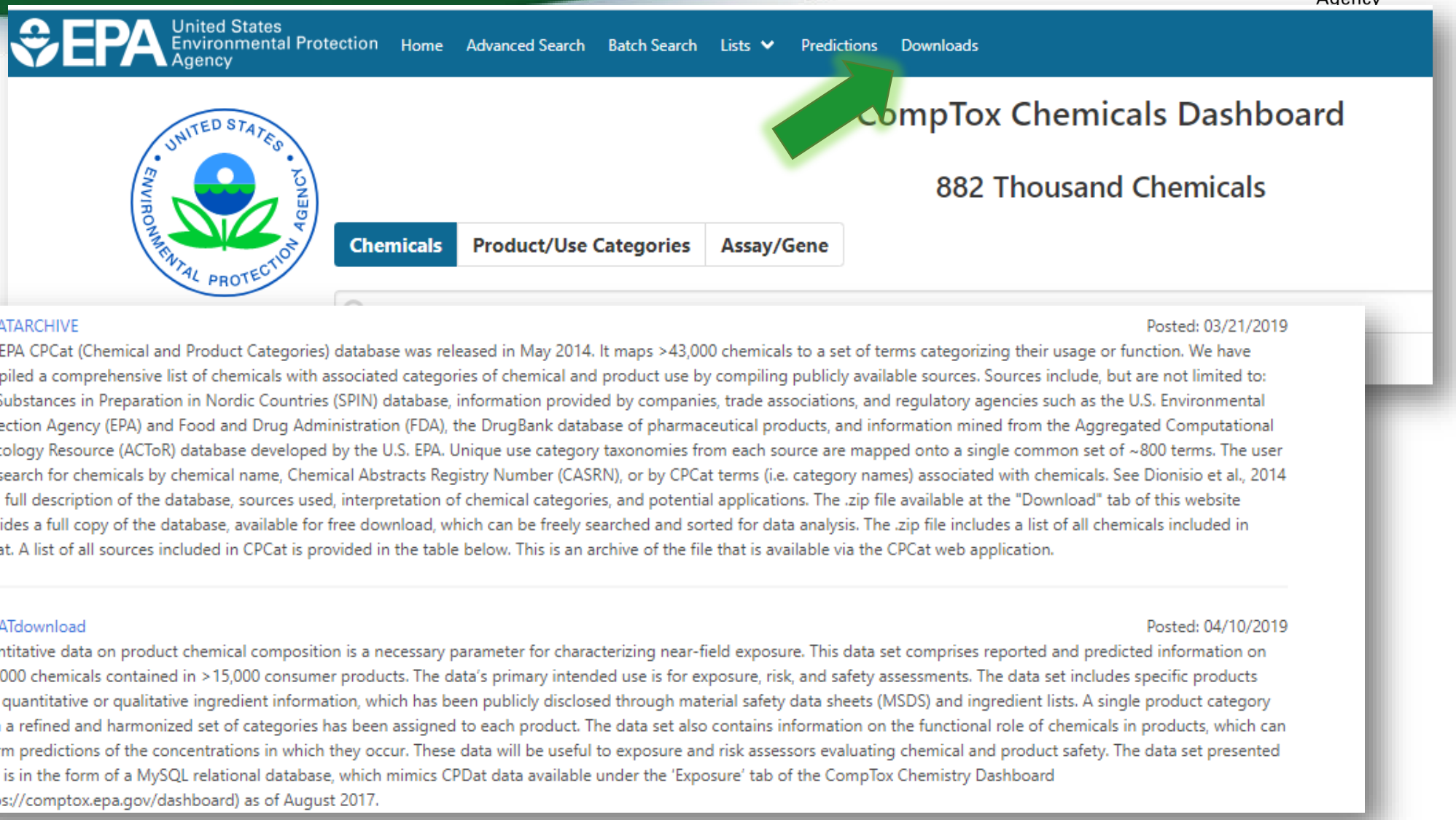
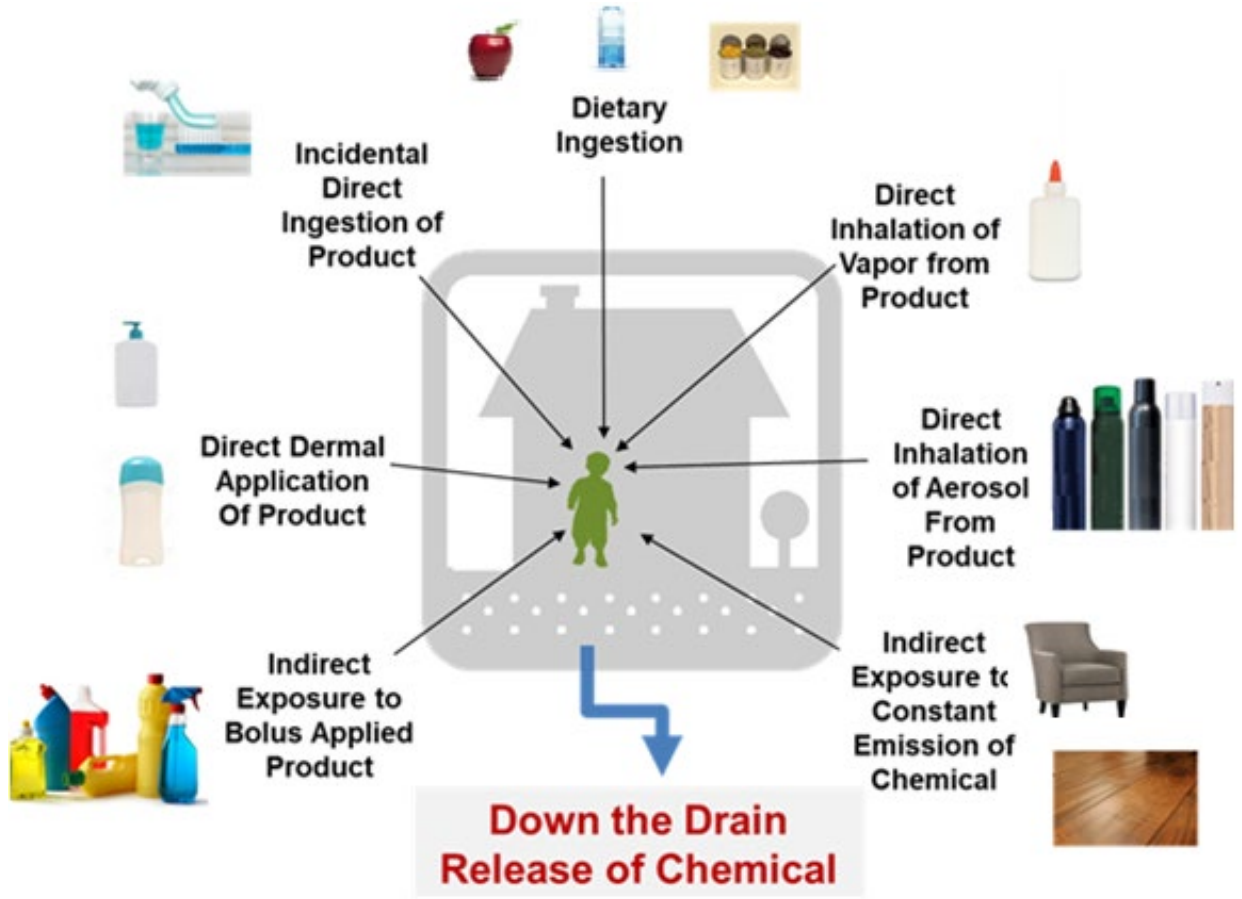


High-Throughput Consumer Exposure Model (SHEDS-HT)

United States Environmental Protection Agency

- CPDat has allowed for rapid parameterization of consumer exposure models, like the High-throughput Stochastic Human Exposure Model (SHEDS-HT)
- SHEDS-HT predicts aggregate population-based human exposures to thousands of commercial chemicals in consumer products, consumer articles, and foods via inhalation, dermal, ingestion, and dietary pathways in a **high-throughput manner**

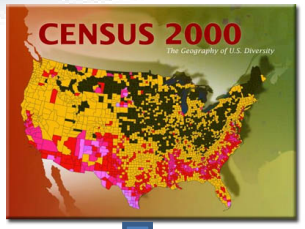
SHEDS-HT



SHEDS-HT

United States Environmental Protection Agency

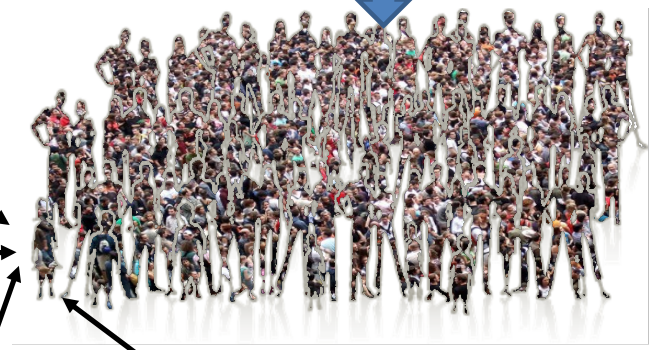
Chemical Residues in Foods



CPDat

Chemical Ingredients and Weight Fractions

Consumer Product Use Patterns



Population Exposures mg/kg-BW/day

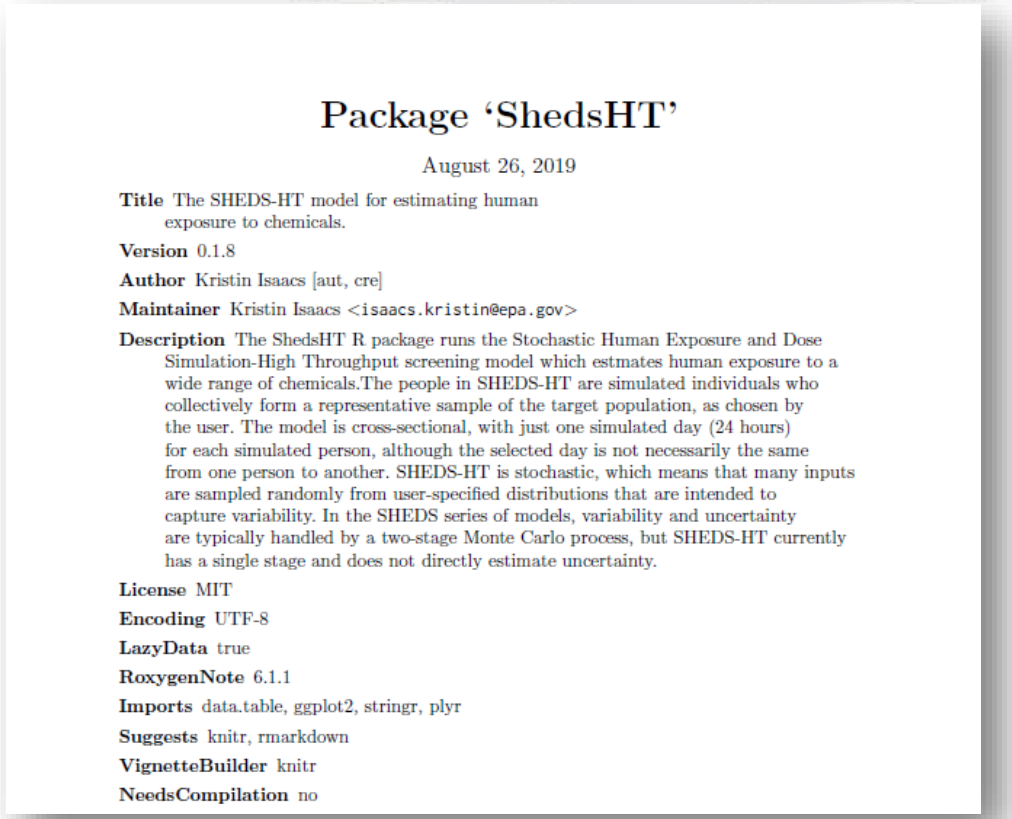
Relevant exposure factors (e.g. weight, bathing and hand washing behaviors, hand-to mouth behaviors)

Daily-level activity diary
- Time spent in microenvironments
- Energy expenditure (ventilation)

Indoor Chemical Emission from Articles

SHEDS-HT

R package 'ShedsHT"



Package 'ShedsHT'

August 26, 2019

Title The SHEDS-HT model for estimating human exposure to chemicals.

Version 0.1.8

Author Kristin Isaacs [aut, cre]

Maintainer Kristin Isaacs <isaacs.kristin@epa.gov>

Description The ShedsHT R package runs the Stochastic Human Exposure and Dose Simulation-High Throughput screening model which estmates human exposure to a wide range of chemicals.The people in SHEDS-HT are simulated individuals who collectively form a representative sample of the target population, as chosen by the user. The model is cross-sectional, with just one simulated day (24 hours) for each simulated person, although the selected day is not necessarily the same from one person to another. SHEDS-HT is stochastic, which means that many inputs are sampled randomly from user-specified distributions that are intended to capture variability. In the SHEDS series of models, variability and uncertainty are typically handled by a two-stage Monte Carlo process, but SHEDS-HT currently has a single stage and does not directly estimate uncertainty.

License MIT

Encoding UTF-8

LazyData true

RoxygenNote 6.1.1

Imports data.table, ggplot2, stringr, plyr

Suggests knitr, rmarkdown

VignetteBuilder knitr

NeedsCompilation no

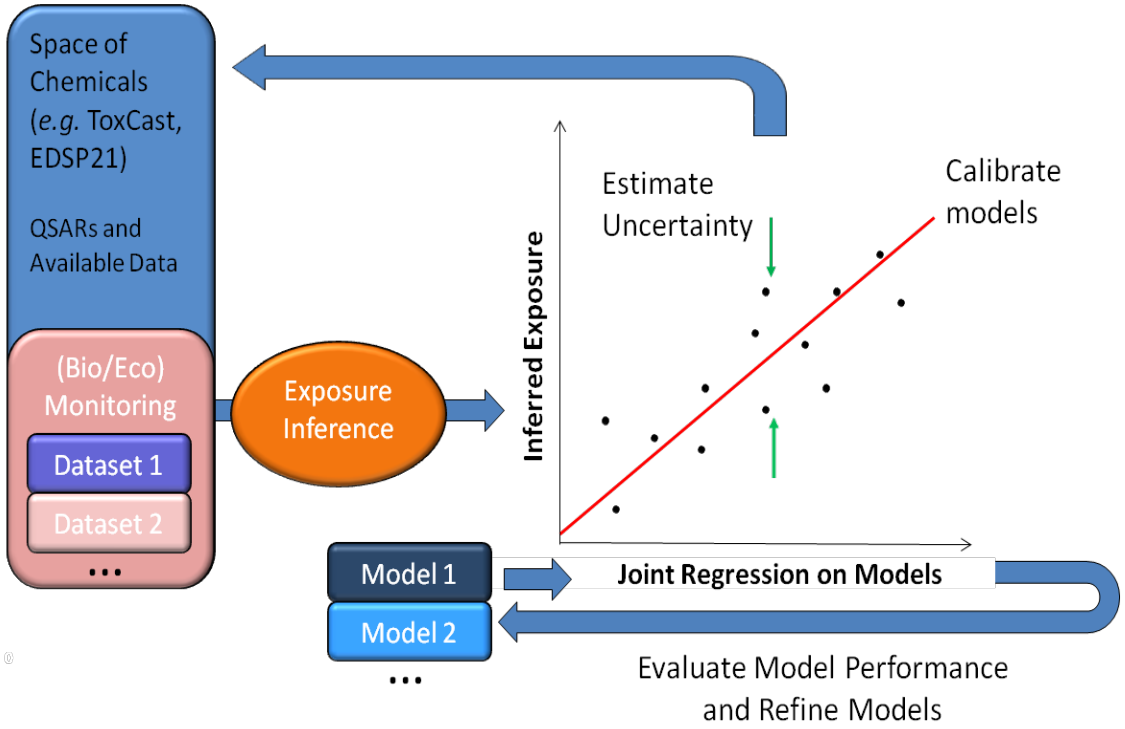
- R Package with help documentation and User's Guide
- Current model release
- Default input files (e.g. population, food diaries, CPDat data in correct form)
- Example run-specific input files
- Training materials
- Example current applications
  - Solvent emissions from consumer products for government inventories
  - Dietary exposures to process-formed chemicals
  - Exposures for chemical-product combinations to inform state decision-making

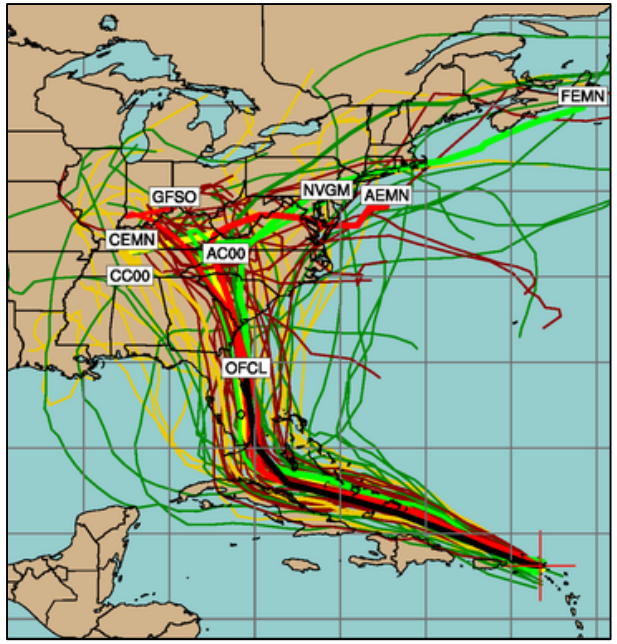
https://github.com/HumanExposure/SHEDSHTRPackage

Consensus Exposure Predictions with the SEEM Framework

United States Environmental Protection Agency

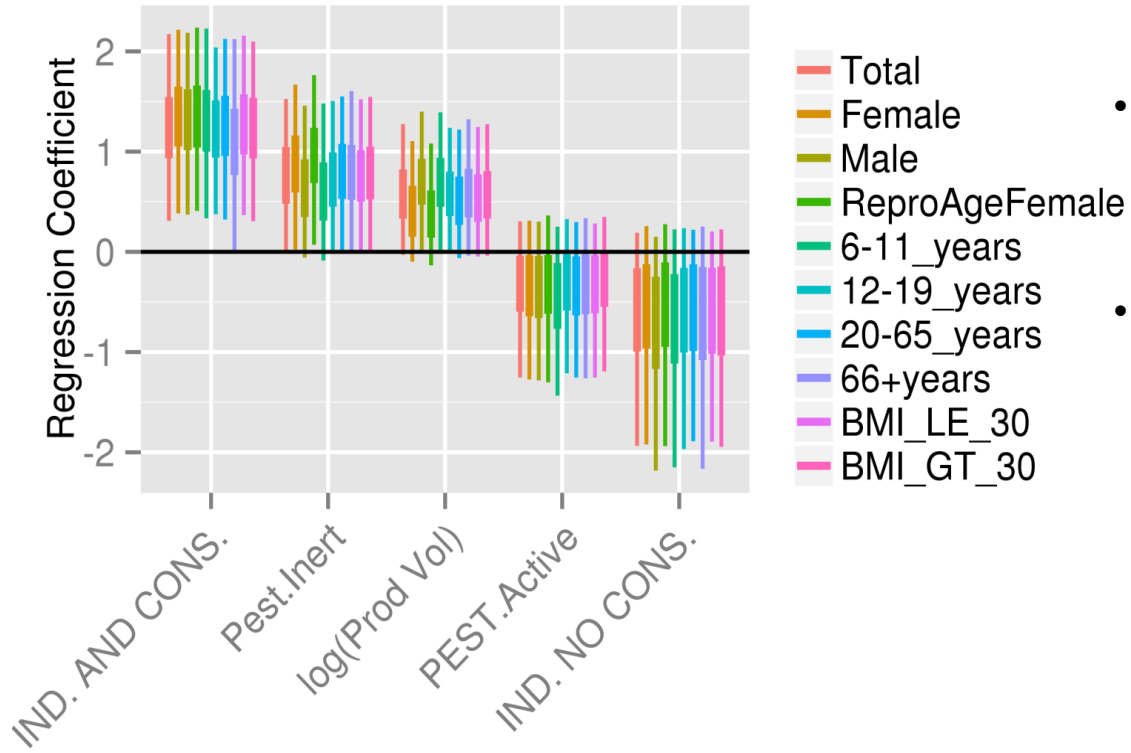
- Different exposure models incorporate **knowledge**, **assumptions**, and **data** (MacLeod et al., 2010)
- We incorporate multiple models (including SHEDS-HT, ExpoDat) into consensus predictions for 1000s of chemicals within the **Systematic Empirical Evaluation of Models (SEEM)** (Wambaugh et al., 2013, 2014, Ring et al., 2019)
- Evaluation is similar to a sensitivity analysis: What models are working? What data are most needed?





Hurricane Path Prediction is an Example of Integrating Multiple Models

Second Generation SEEM: Heuristics of Exposure



Wambaugh *et al.* (2014)

- Use and production volume descriptors used to build parsimonious model for inferred exposure
- Five descriptors explain roughly 50% of the chemical to chemical variability in median NHANES exposure rates
- Same five predictors work for all NHANES demographic groups analyzed – stratified by age, sex, and body-mass index:
  - Industrial and Consumer use
  - Pesticide Inert
  - Pesticide Active
  - Industrial but no Consumer use
  - Production Volume
- What we are really doing is identifying chemical exposure pathway

Evaluation Data for SEEM: Exposures Inferred from NHANES

United States Environmental Protection Agency

- Annual survey, data released on 2-year cycle
- Separate evaluations can be done for various demographics
- ~2000 individuals per chemical, with statistical weights allowing inference for larger U.S. populations
- To date, we have used this to draw inference about median exposure rates

National Health and Nutrition Examination Survey

Urinary Bisphenol A (2,2-*bis*[4-Hydroxyphenyl] propane)

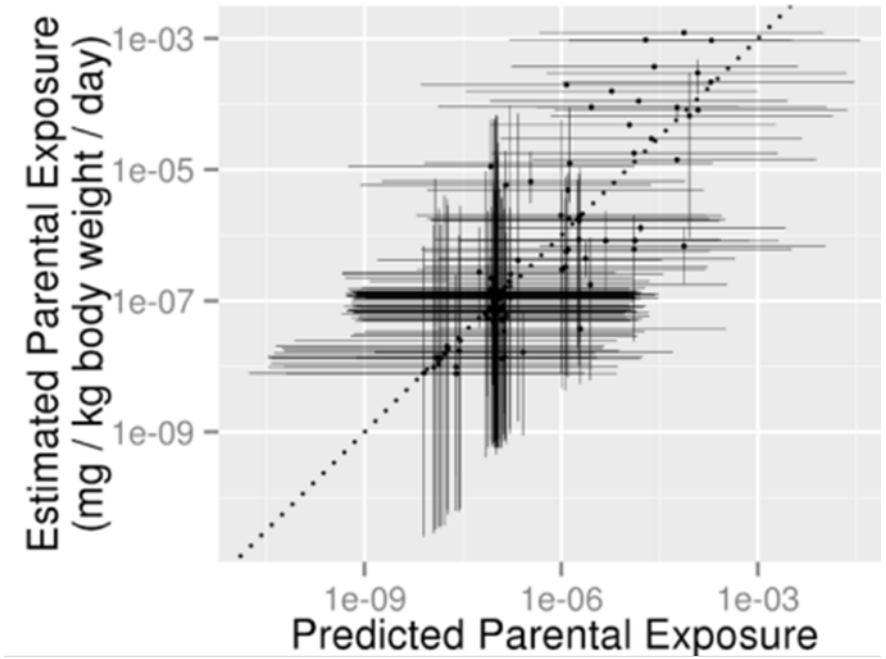
Geometric mean and selected percentiles of urine concentrations (in µg/L) for the U.S. populatio and Nutrition Examination Survey.

	Survey years	Geometric mean (95% conf. interval)	Selected percentiles (95% confidence interval) 50th	75th	90th
Total	03-04	2.64 (2.38-2.94)	2.80 (2.50-3.10)	5.50 (5.00-6.20)	10.6 (9.40-
	05-06	1.90 (1.79-2.02)	2.00 (1.90-2.00)	3.70 (3.50-3.90)	7.00 (6.40-
	07-08	2.08 (1.92-2.26)	2.10 (1.90-2.30)	4.10 (3.60-4.60)	7.70 (6.80-
Age group					
6-11 years	03-04	3.55 (2.95-4.29)	3.80 (2.70-5.00)	6.90 (6.00-8.30)	12.6 (9.50-
	05-06	2.86 (2.52-3.24)	2.70 (2.30-2.90)	5.00 (4.40-5.80)	13.5 (9.30-
	07-08	2.46 (2.20-2.75)	2.40 (1.90-3.00)	4.50 (3.70-5.50)	7.00 (6.30-
12-19 years	03-04	3.74 (3.31-4.22)	4.30 (3.60-4.60)	7.80 (6.50-9.00)	13.5 (11.8-
	05-06	2.42 (2.18-2.68)	2.40 (2.10-2.70)	4.30 (3.90-5.20)	8.40 (6.50-
	07-08	2.44 (2.14-2.78)	2.30 (2.10-2.60)	4.40 (3.70-5.50)	9.70 (7.30-
20 years and older	03-04	2.41 (2.15-2.72)	2.60 (2.30-2.80)	5.10 (4.50-5.70)	9.50 (8.10-
	05-06	1.75 (1.62-1.89)	1.80 (1.70-2.00)	3.40 (3.10-3.70)	6.40 (5.80-
	07-08	1.99 (1.82-2.18)	2.00 (1.80-2.30)	3.90 (3.40-4.60)	7.40 (6.60-

CDC, Fourth National Exposure Report (2011)

Second Generation SEEM: Heuristics of Exposure

$R^2 \sim 0.5$



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- What we are really doing is identifying chemical exposure pathway

Wambaugh et al., 2014

SEEM3 Collaboration

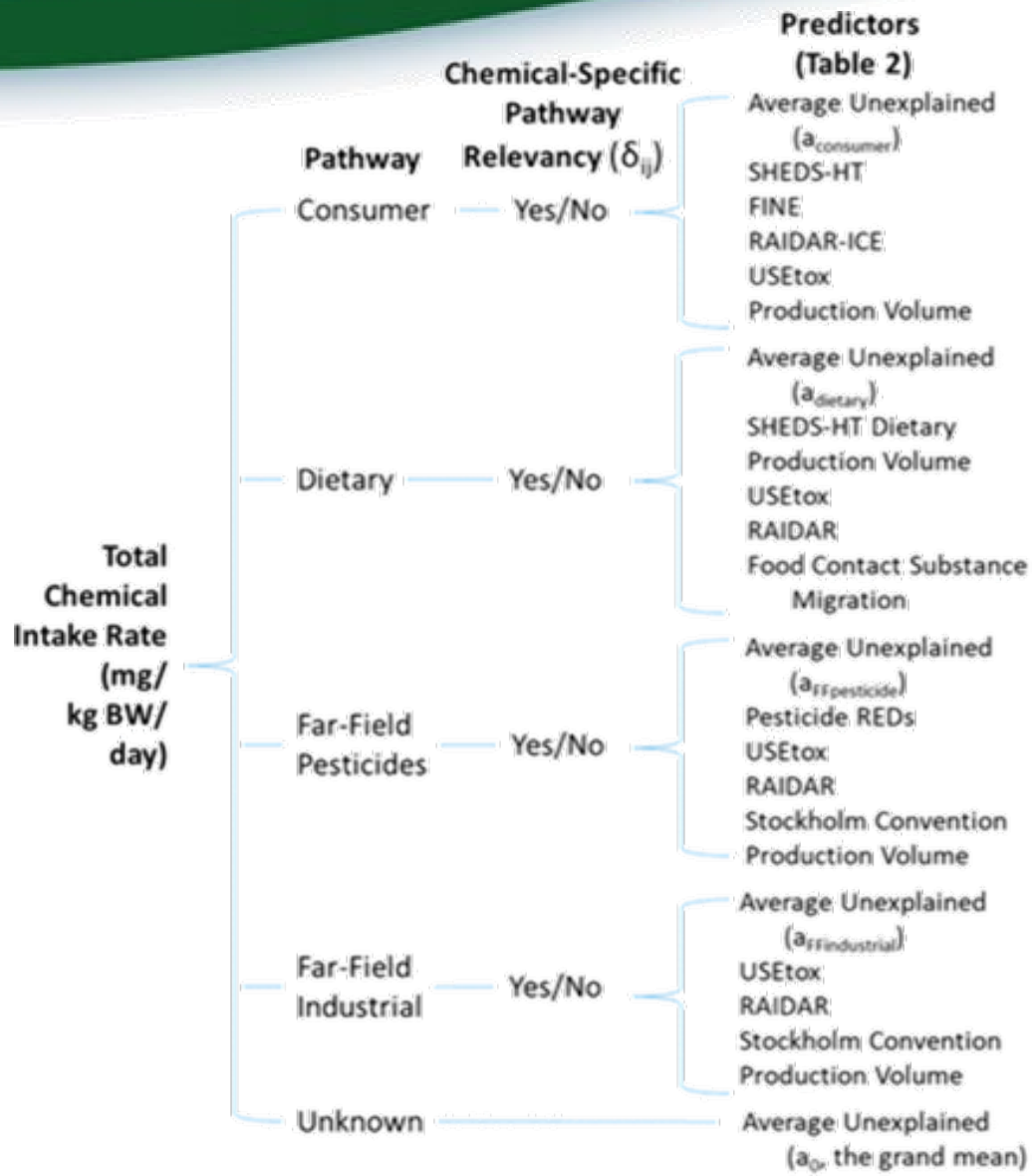
Jon Arnot, Deborah H. Bennett, Peter P. Egeghy, Peter Fantke, Lei Huang, Kristin K. Isaacs, Olivier Jolliet, Hyeong-Moo Shin, Katherine A. Phillips, Caroline Ring, R. Woodrow Setzer, John F. Wambaugh, Johnny Westgate

Predictor	Reference(s)	Chemicals Predicted	Pathways
EPA Inventory Update Reporting and Chemical Data Reporting (CDR) (2015)	US EPA (2018)	7856	All
Stockholm Convention of Banned Persistent Organic Pollutants (2017)	Lallas (2001)	248	Far-Field Industrial and Pesticide
EPA Pesticide Reregistration Eligibility Documents (REDs) Exposure Assessments (Through 2015)	Wetmore et al. (2012, 2015)	239	Far-Field Pesticide
United Nations Environment Program and Society for Environmental Toxicology and Chemistry toxicity model (USEtox) Industrial Scenario (2.0)	Rosenbaum et al. (2008)	8167	Far-Field Industrial
USEtox Pesticide Scenario (2.0)	Fantke et al. (2011, 2012, 2016)	940	Far-Field Pesticide
Risk Assessment IDentification And Ranking (RAIDAR) Far-Field (2.02)	Arnot et al. (2008)	8167	Far-Field Pesticide
EPA Stochastic Human Exposure Dose Simulator High Throughput (SHEDS-HT) Near-Field Direct (2017)	Isaacs (2017)	7511	Far-Field Industrial and Pesticide
SHEDS-HT Near-field Indirect (2017)	Isaacs (2017)	1119	Residential
Fugacity-based INdoor Exposure (FINE) (2017)	Bennett et al. (2004), Shin et al. (2012)	645	Residential
RAIDAR-ICE Near-Field (0.803)	Arnot et al., (2014), Zhang et al. (2014)	1221	Residential
USEtox Residential Scenario (2.0)	Jolliet et al. (2015), Huang et al. (2016,2017)	615	Residential
USEtox Dietary Scenario (2.0)	Jolliet et al. (2015), Huang et al. (2016), Ernstoff et al. (2017)	8167	Dietary

Ring et al., 2018

SEEM3 Considers Pathway!

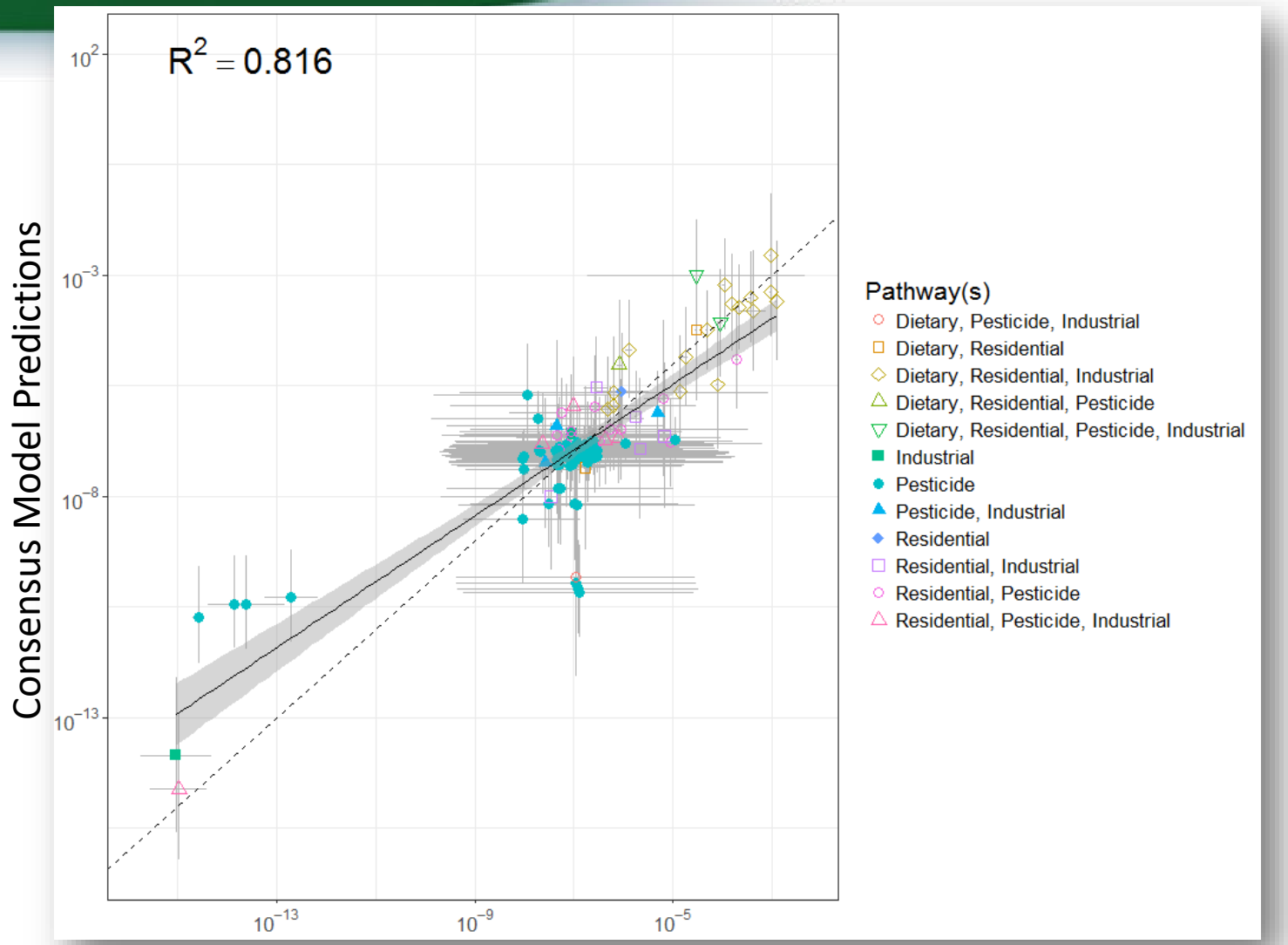
We organize the models by the exposure pathways they cover!



Ring et al., 2018

Pathway-Based Consensus Modeling

United States Environmental Protection Agency



Ring et al., 2018

Predicting Relevant Pathways for a Chemical

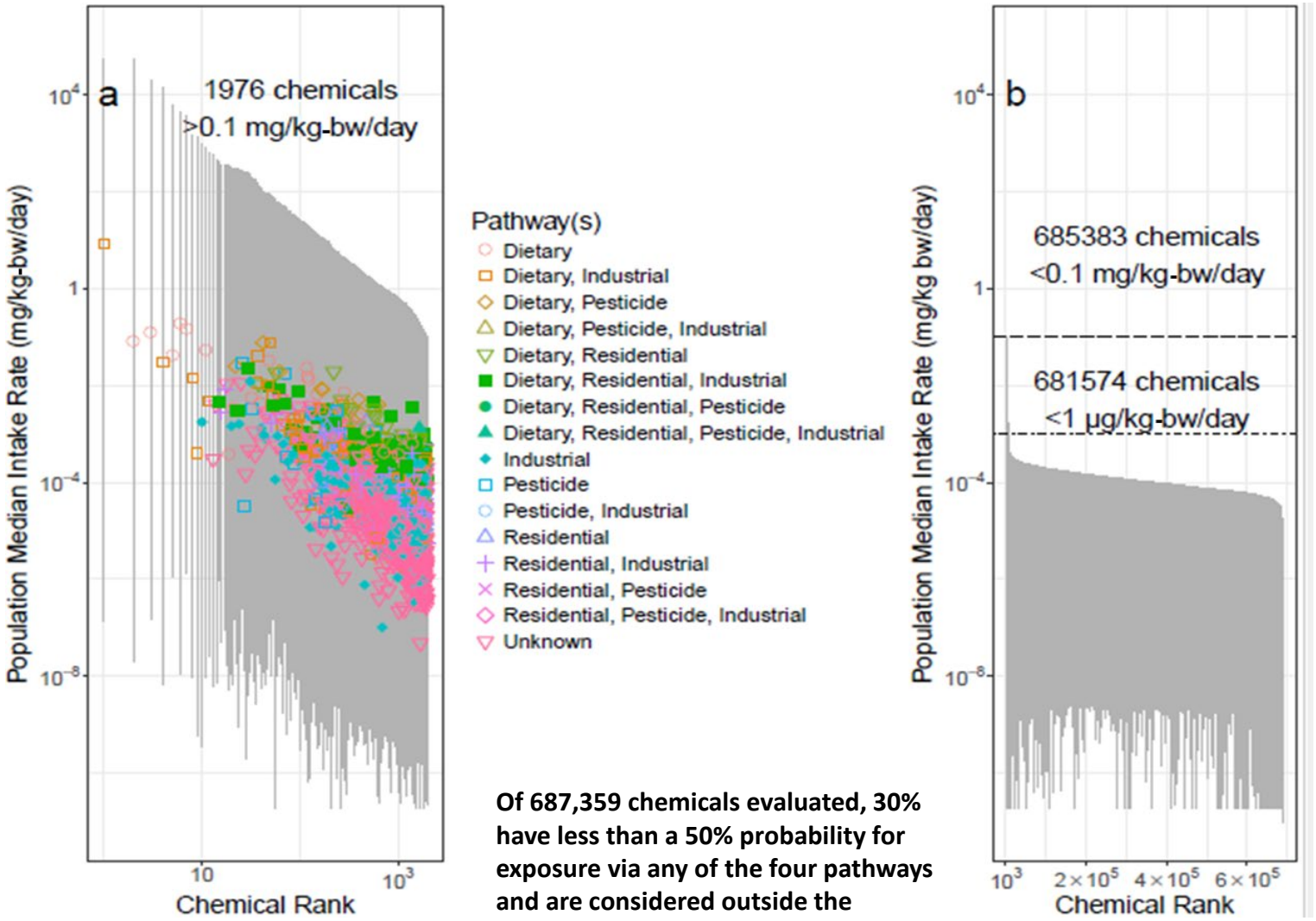
United States Environmental Protection Agency

We use the method of Random Forests to relate chemical structure and properties to exposure pathway

	NHANES Chemicals Positives		Negatives	OOB Error Rate	Positives Error Rate	Balanced Accuracy	Sources of Positives	Sources of Negatives
Dietary	24	2523	8865	27	32	73	FDA CEDI, ExpoCast, CPDat (Food, Food Additive, Food Contact), NHANES Curation	Pharmapendium, CPDat (non-food), NHANES Curation
Near-Field	**49**	1622	567	26	24	74	CPDat (consumer_use, building_material), ExpoCast, NHANES Curation	CPDat (Agricultural, Industrial), FDA CEDI, NHANES Curation
Far-Field Pesticide	**94**	1480	6522	21	36	80	REDs, Swiss Pesticides, Stockholm Convention, CPDat (Pesticide), NHANES Curation	Pharmapendium, Industrial Positives, NHANES Curation
Far Field Industrial	**42**	5089	2913	19	16	81	CDR HPV, USGS Water Occurrence, NORMAN PFAS, Stockholm Convention, CPDat (Industrial, Industrial_Fluid), NHANES Curation	Pharmapendium, Pesticide Positives, NHANES Curation

Ring et al., 2018

Consensus Modeling of Median Chemical Intake

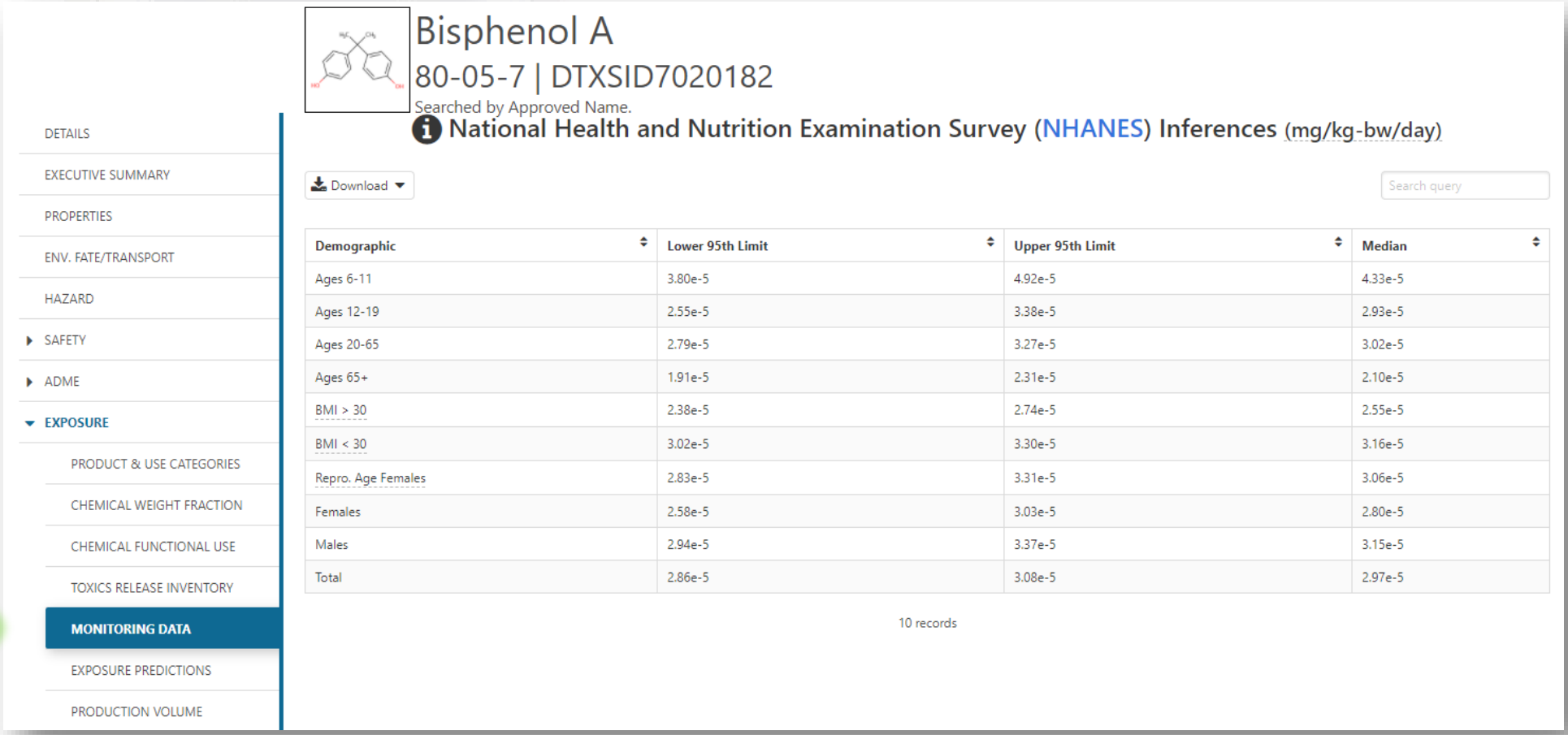


Of 687,359 chemicals evaluated, 30% have less than a 50% probability for exposure via any of the four pathways and are considered outside the "domain of applicability"

Ring et al., 2018

Exposure Predictions in the CompTox Chemicals Dashboard

United States Environmental Protection Agency



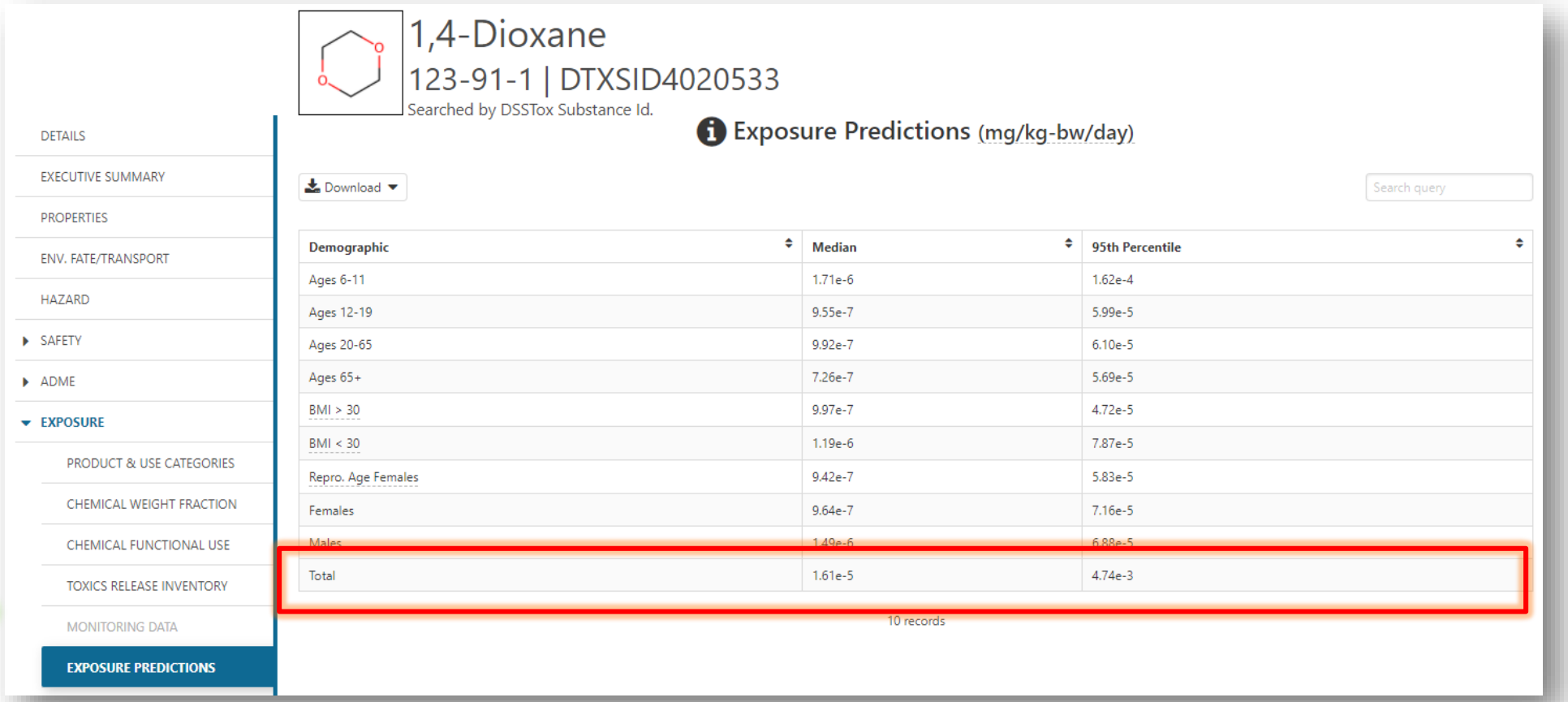
Demographic	Lower 95th Limit	Upper 95th Limit	Median
Ages 6-11	3.80e-5	4.92e-5	4.33e-5
Ages 12-19	2.55e-5	3.38e-5	2.93e-5
Ages 20-65	2.79e-5	3.27e-5	3.02e-5
Ages 65+	1.91e-5	2.31e-5	2.10e-5
BMI > 30	2.38e-5	2.74e-5	2.55e-5
BMI < 30	3.02e-5	3.30e-5	3.16e-5
Repro. Age Females	2.83e-5	3.31e-5	3.06e-5
Females	2.58e-5	3.03e-5	2.80e-5
Males	2.94e-5	3.37e-5	3.15e-5
Total	2.86e-5	3.08e-5	2.97e-5

These are the exposure inferences used to calibrate the SEEM models.

Exposure Predictions in the CompTox Chemicals Dashboard

United States Environmental Protection Agency

What about a chemical without biomonitoring data?



- SEEM3 Predictions for Total Population
- SEEM2 Predictions for Other Cohorts

Summary

- Chemical use data are critical for understanding exposure pathways, parameterizing high-throughput exposure models, and extrapolating information to data-poor chemicals.
- The results from multiple pathway-specific exposure models can be integrated into consensus predictions for median population exposure.
- The ExpoCast project is working to develop chemical use information and exposure predictions for thousands of chemicals, and to provide these data and tools via the Dashboard or other public platforms.
- These “New Approach Methodologies” for exposure ultimately facilitate risk-based prioritization of thousands of chemicals when integrated with *in vitro* bioactive concentrations that have been converted to an equivalent intake exposure.

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ExpoCast Project (Exposure Forecasting)

CCTE

Linda Adams
Miyuki Breen*
Alex Chao*
Dan Dawson*
Mike Devito
Kathie Dionisio
Christopher Ecklund
Marina Evans
Peter Egeghy
Michael-Rock Goldsmith
Chris Grulke
Mike Hughes
Kristin Isaacs
Richard Judson
Jen Korol-Bexell*
Anna Kreutz*
Charles Lowe*
Seth Newton
Katherine Phillips
Paul Price
Tom Purucker
Ann Richard
Caroline Ring
Marci Smeltz*
Jon Sobus
Risa Sayre*
Mark Sfeir*
Mark Strynar
Zach Stanfield*
Rusty Thomas
Mike Tornero-Velez
Elin Ulrich
Dan Vallero
Taylor Wall*
John Wambaugh
Barbara Wetmore
Antony Williams

CEMM

Xiaoyu Liu

CPHEA

Jane Ellen Simmons
Jeff Minucci

CESER

David Meyer
Gerardo Ruiz-Mercado
Wes Ingwersen

***Trainees**

Collaborators

Arnot Research and Consulting
Jon Arnot
Johnny Westgate
Institut National de l'Environnement et des Risques (INERIS)
Frederic Bois
Integrated Laboratory Systems
Kamel Mansouri
National Toxicology Program
Steve Ferguson
Nisha Sipes
Ramboll
Harvey Clewell
Silent Spring Institute
Robin Dodson
Southwest Research Institute
Alice Yau
Kristin Favela
Summit Toxicology
Lesa Aylward
Technical University of Denmark
Peter Fantke
Tox Strategies
Miyoung Yoon
Unilever
Beate Nicol
Cecilie Rendal
Ian Sorrell
United States Air Force
Heather Pangburn
Matt Linakis
University of California, Davis
Deborah Bennett
University of Michigan
Olivier Jolliet
University of Texas, Arlington
Hyeong-Moo Shin