

Exposure Data and Gap-filling Methods

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Disclaimer: The views expressed in this presentation are those of the authors and do not necessarily reflect the views or policies of the U.S. Environmental Protection Agency.

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Summit Toxicology

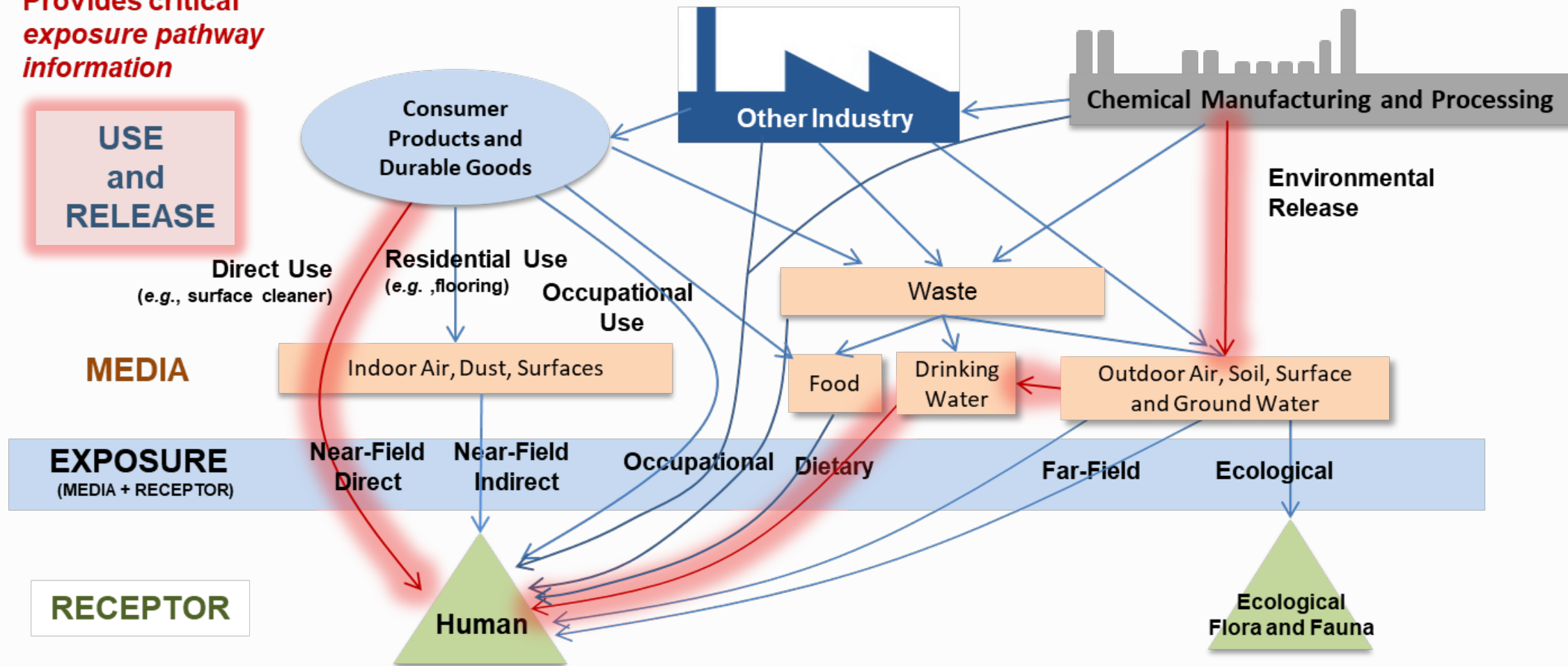
Lisa Aylward

ICF International

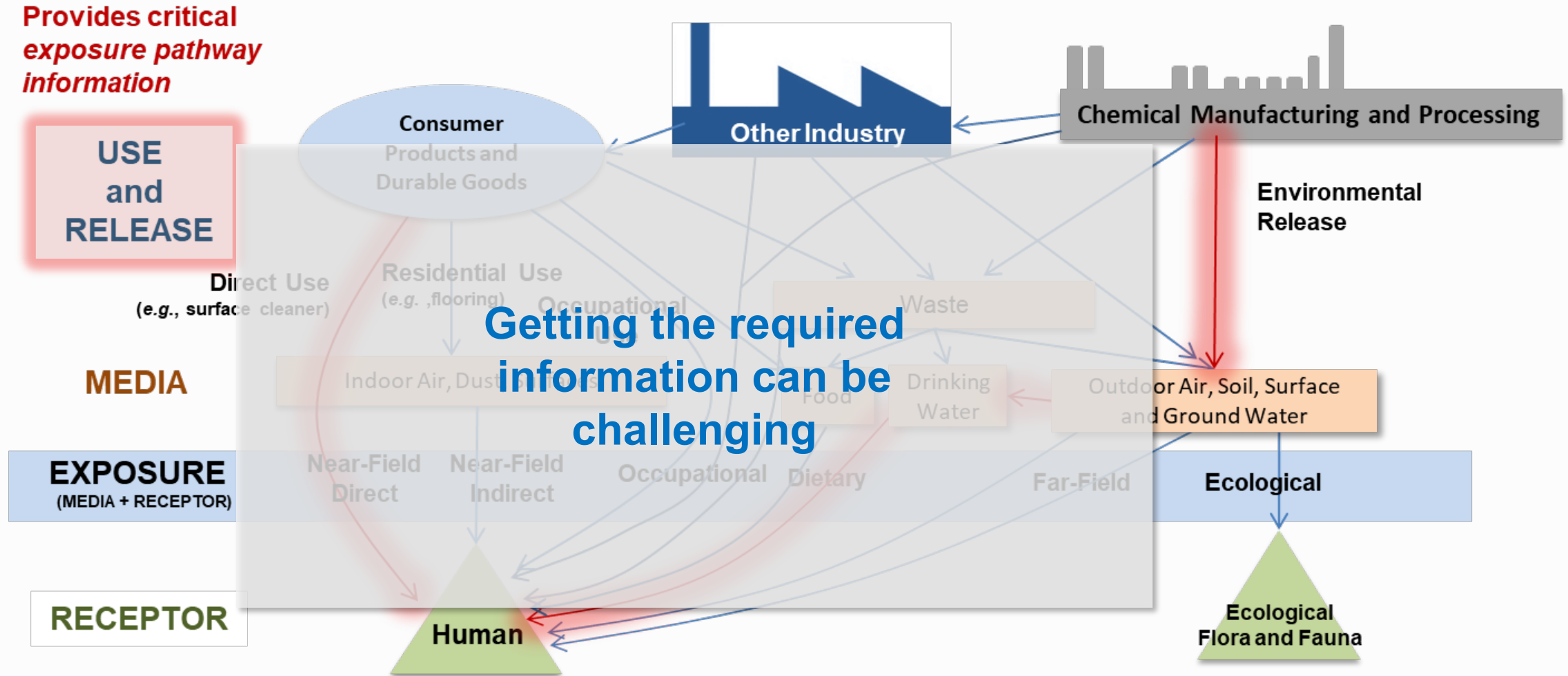
Tao Hong

Information Required for Exposure Estimations

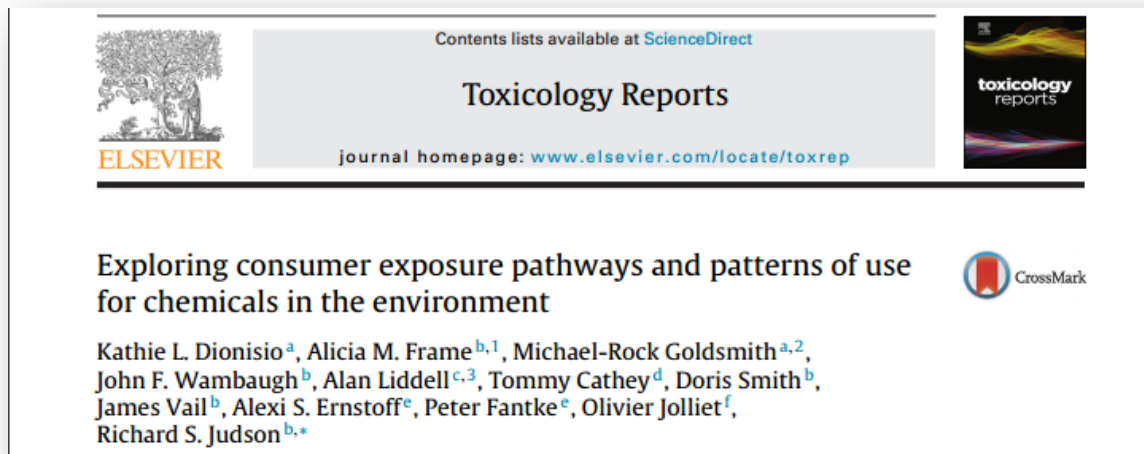
**Provides critical
exposure pathway
information**



Information Required for Exposure Estimations



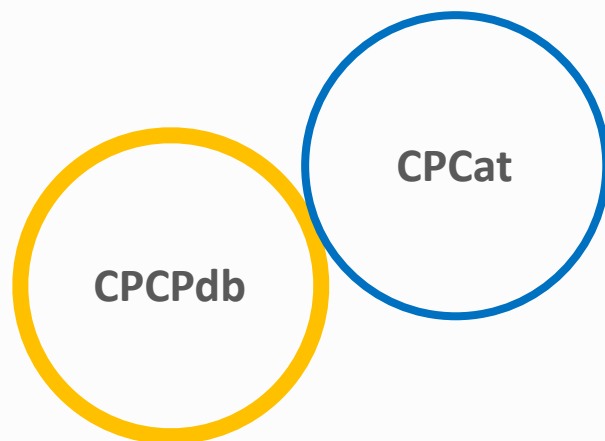
Chemical Product Categories Database (CPCat)



Broad categorization of chemical use

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

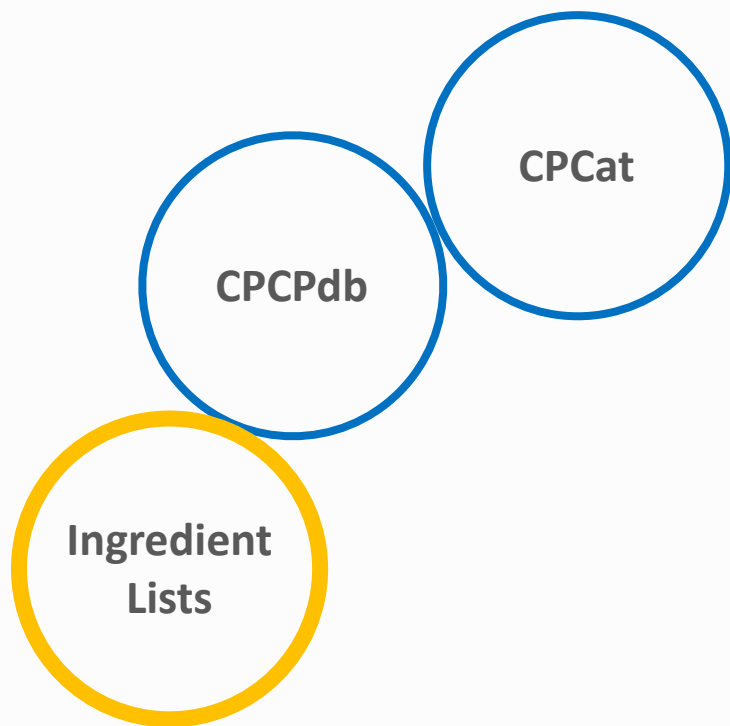
Chemical Products Chemical Profiles Database (CPCPdb)



MSDS-based composition information

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

Consumer Product Ingredient Lists



Ingredient Lists

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

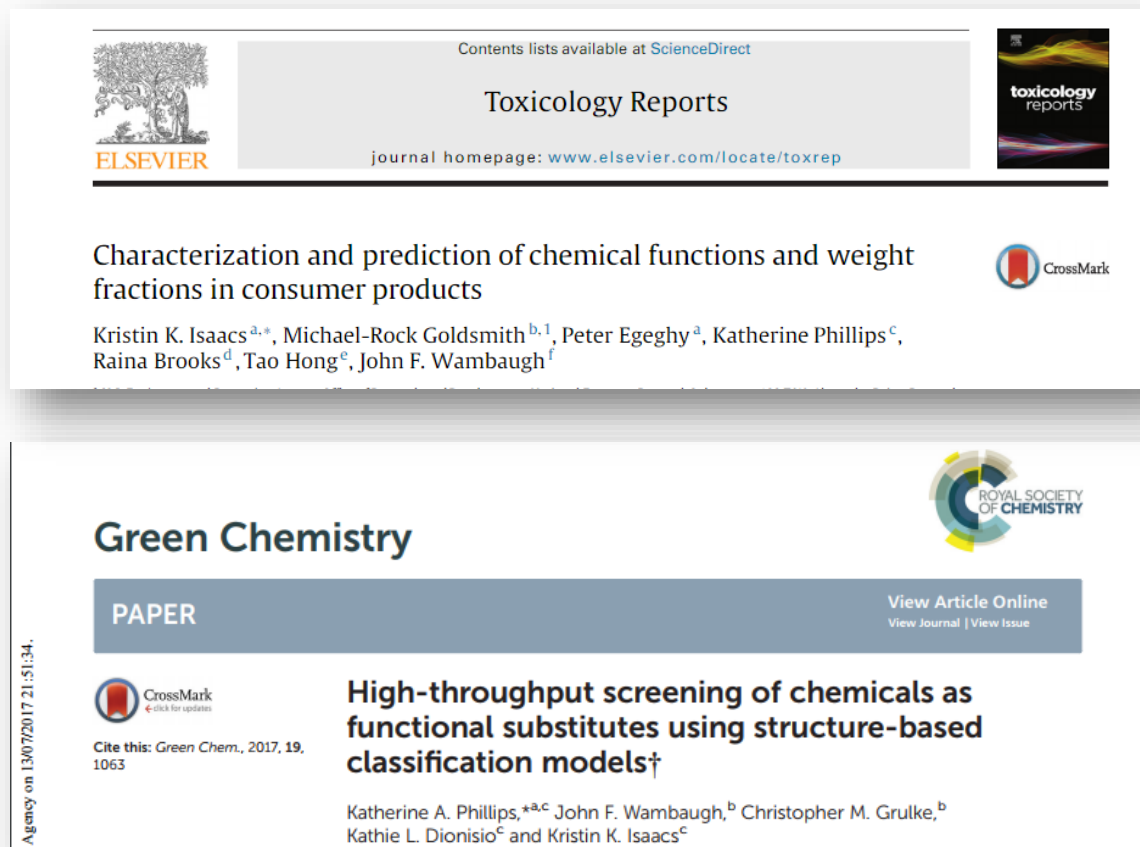
Chemical Functional Use

CPCat

CPCPdb

Ingredient
Lists

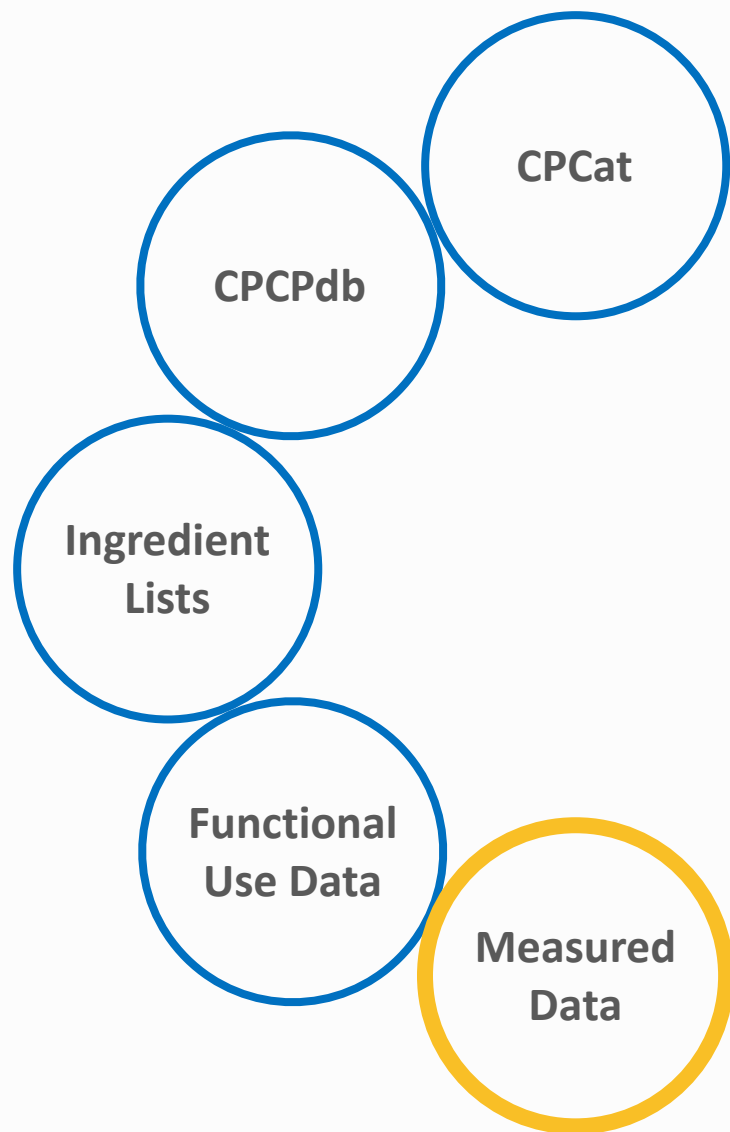
Functional
Use Data



Categorization by functional use

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

Suspect Screening/Non-targeted Analysis Data



ENVIRONMENTAL
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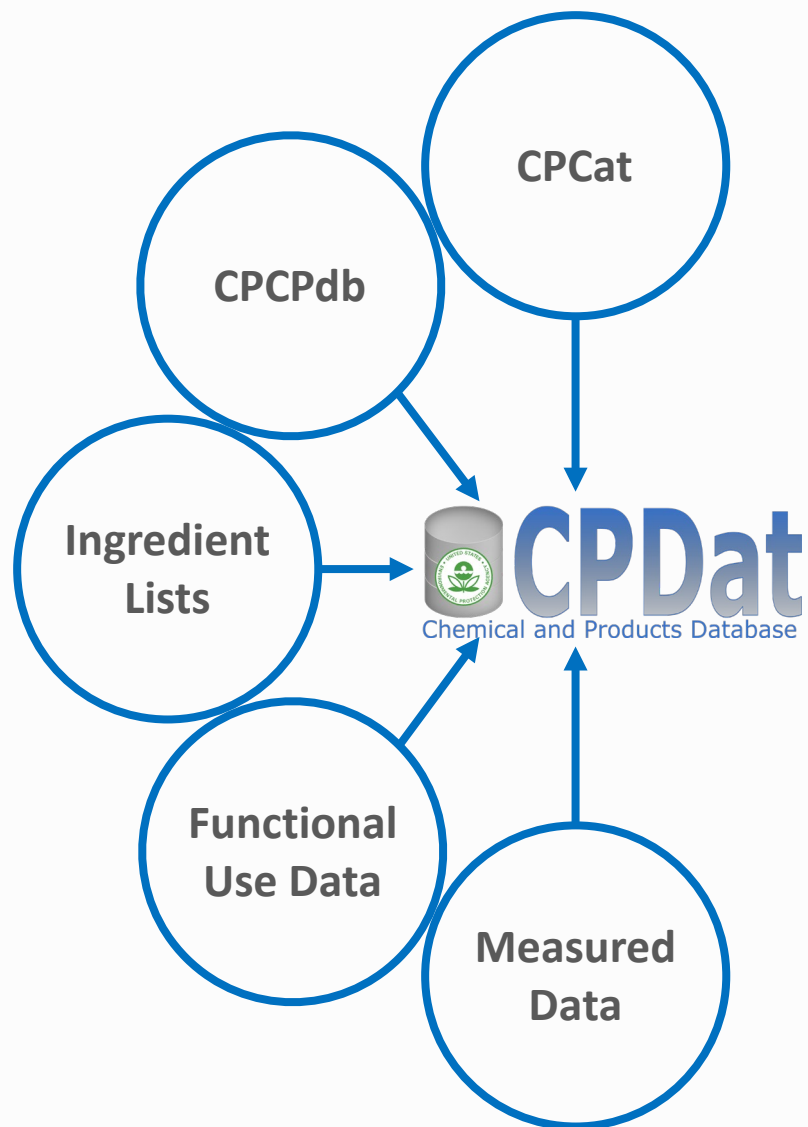
Suspect Screening Analysis of Chemicals in Consumer Products

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^{*,||}

Measurement of chemicals in consumer products

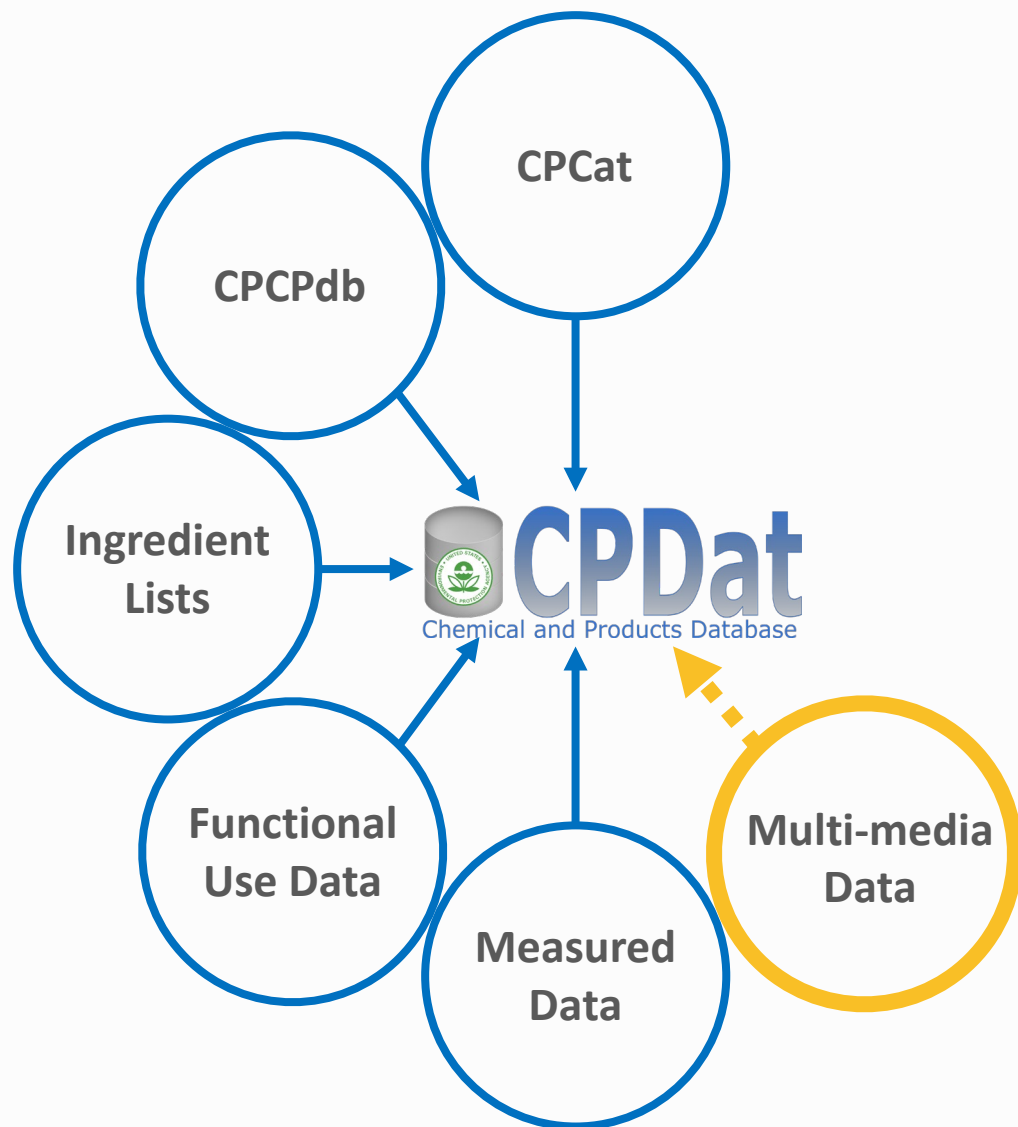
- Estimates of weight fractions from measurements
- Confirmed presence
- Tentative identification

The Chemicals and Products Database



Organization of many separate, but related, data sets into a single, publicly accessible and searchable database.

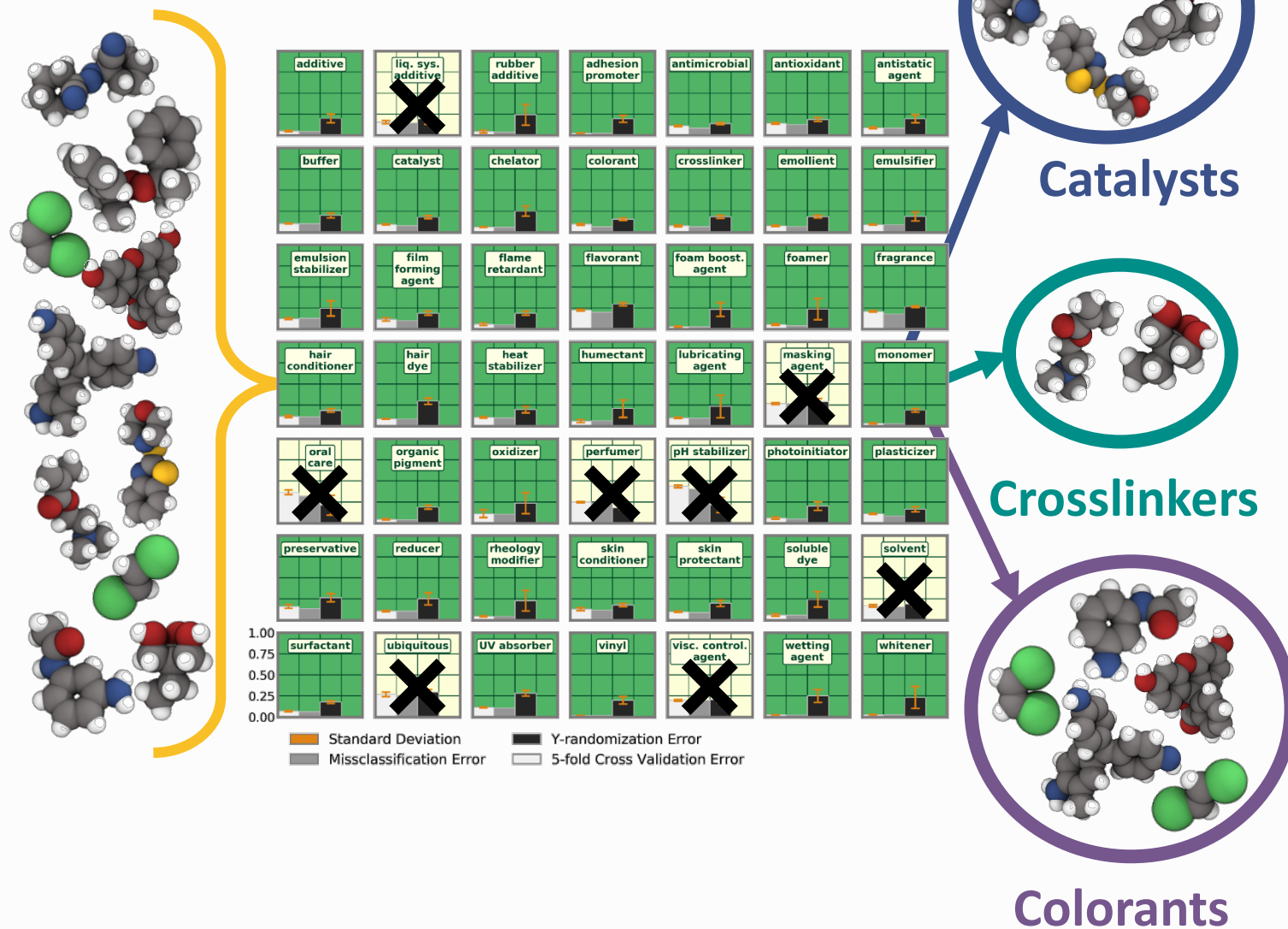
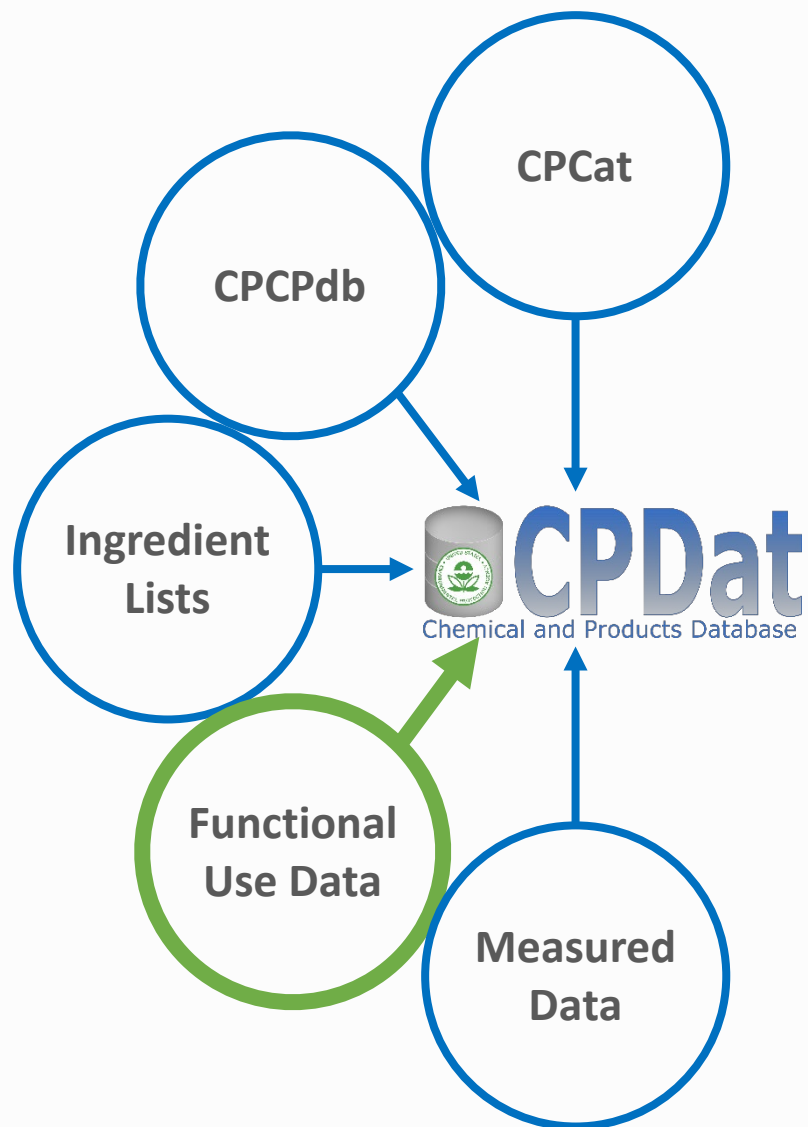
The Chemicals and Products Database



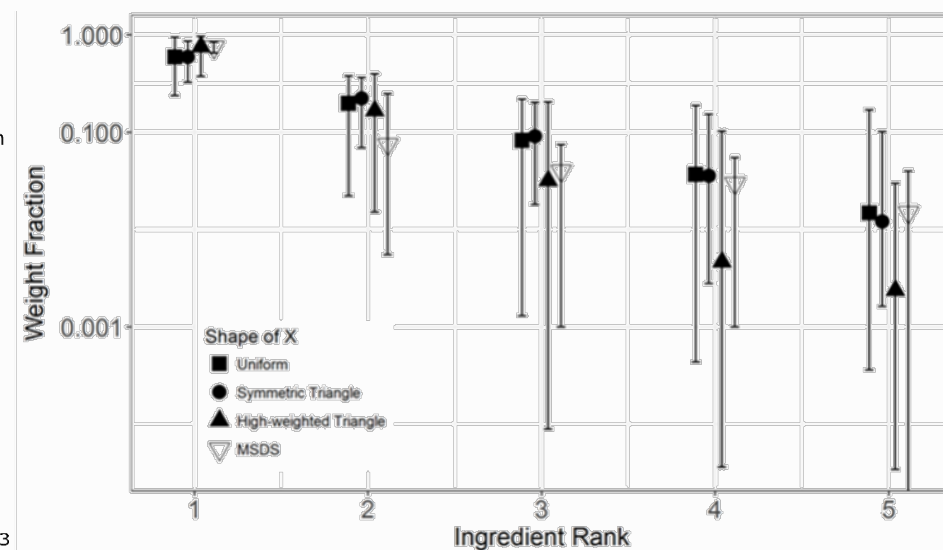
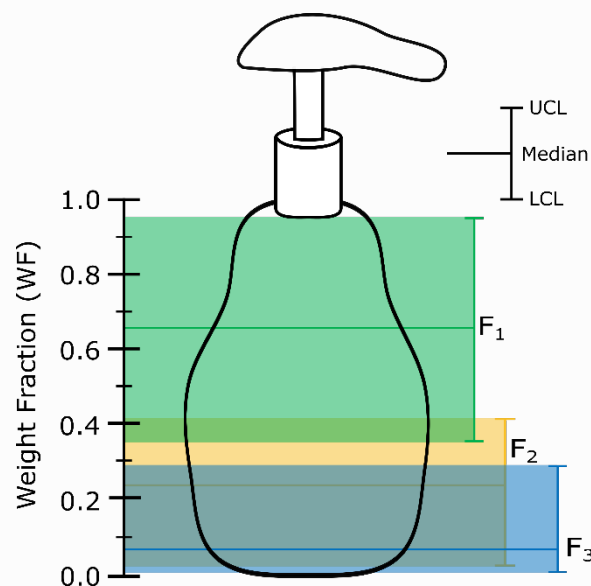
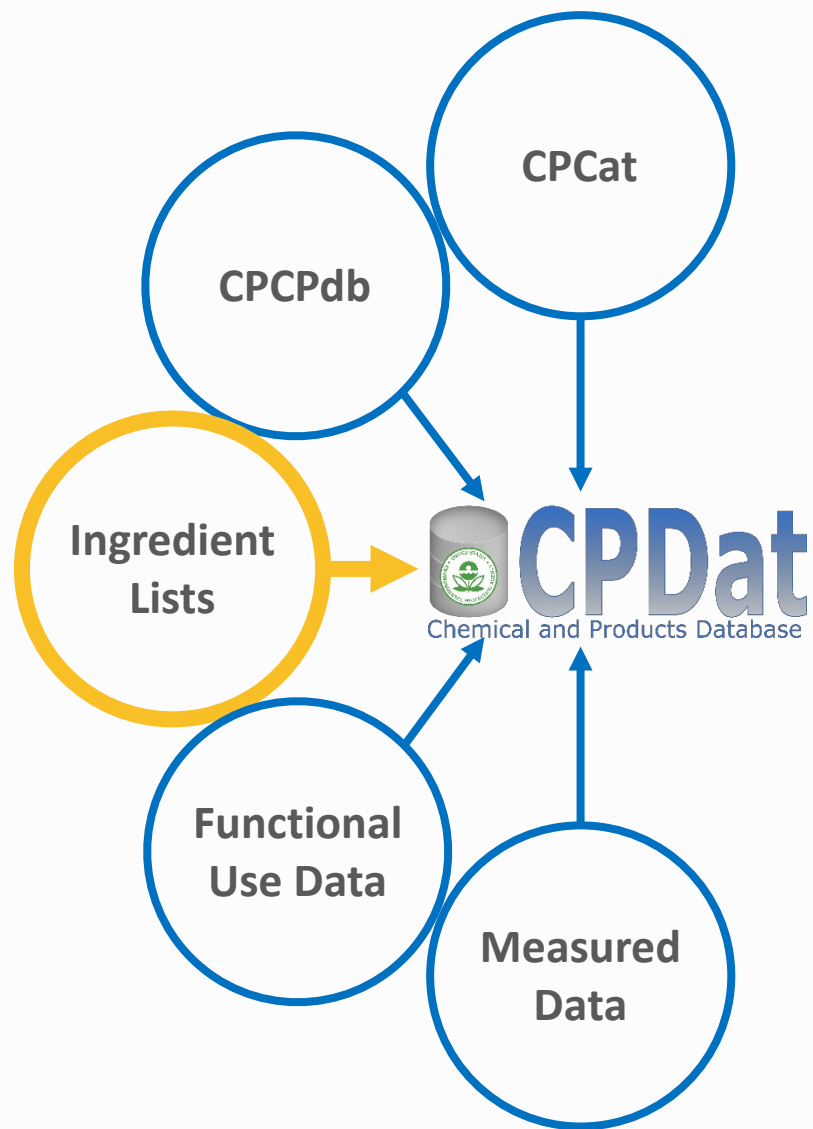
Multi-media Data

- contains data on which chemicals have previously been identified in targeted studies in specific media
- data is collected and reviewed from published studies and will be added to future versions of CPDat

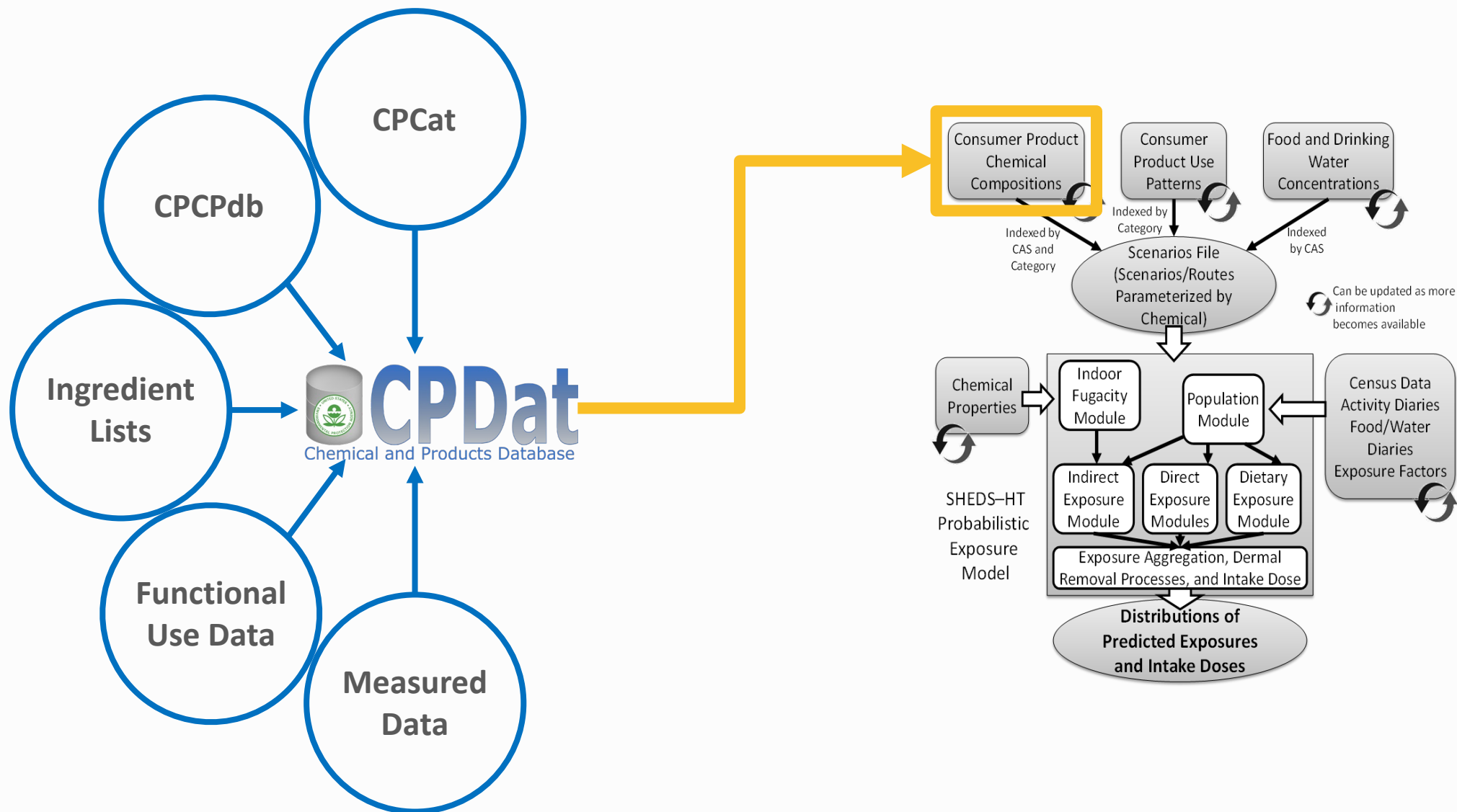
Quantitative Structure-Use Relationships (QSURs)



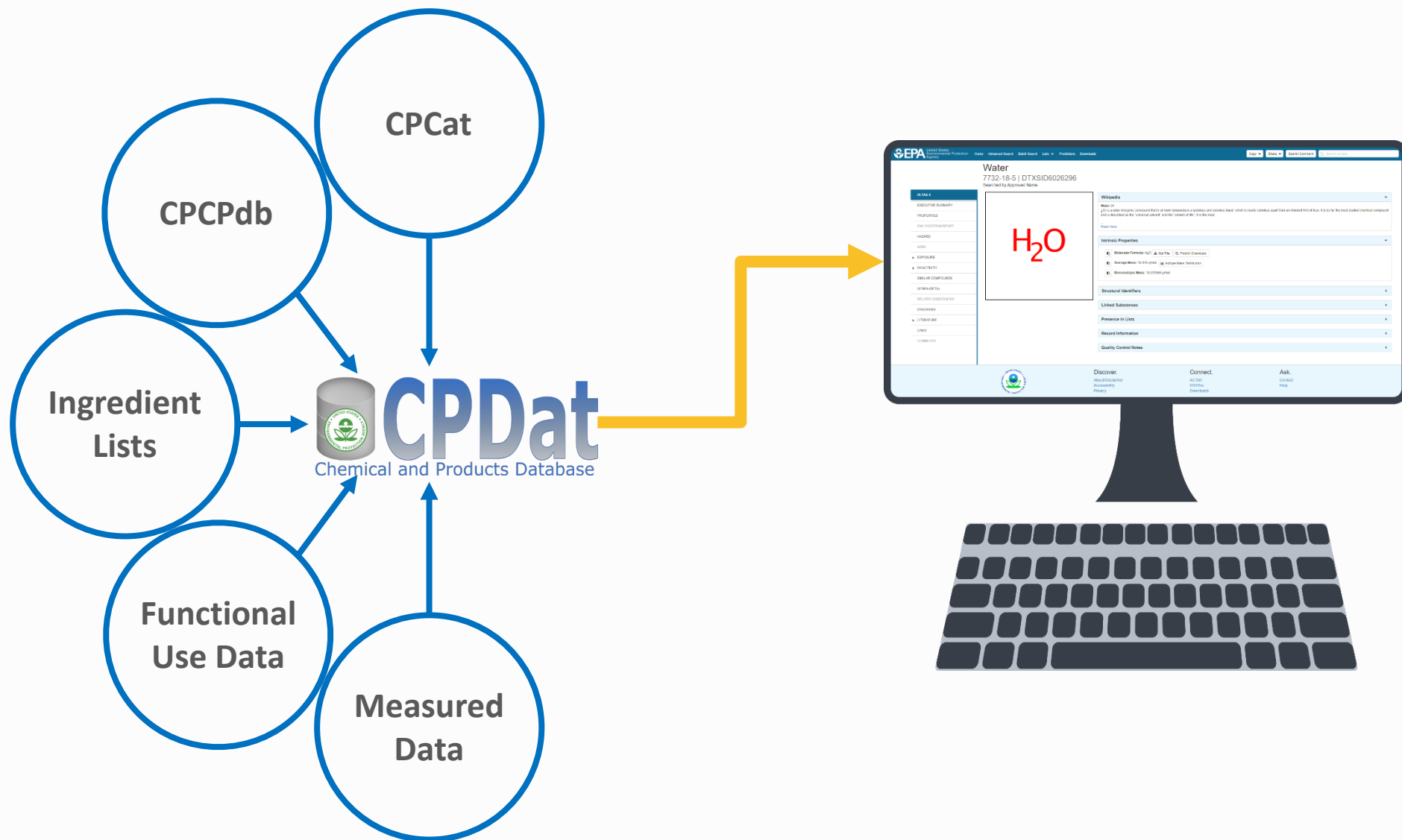
Ingredient Weight Fraction Prediction



CPDat aids Exposure Forecasting

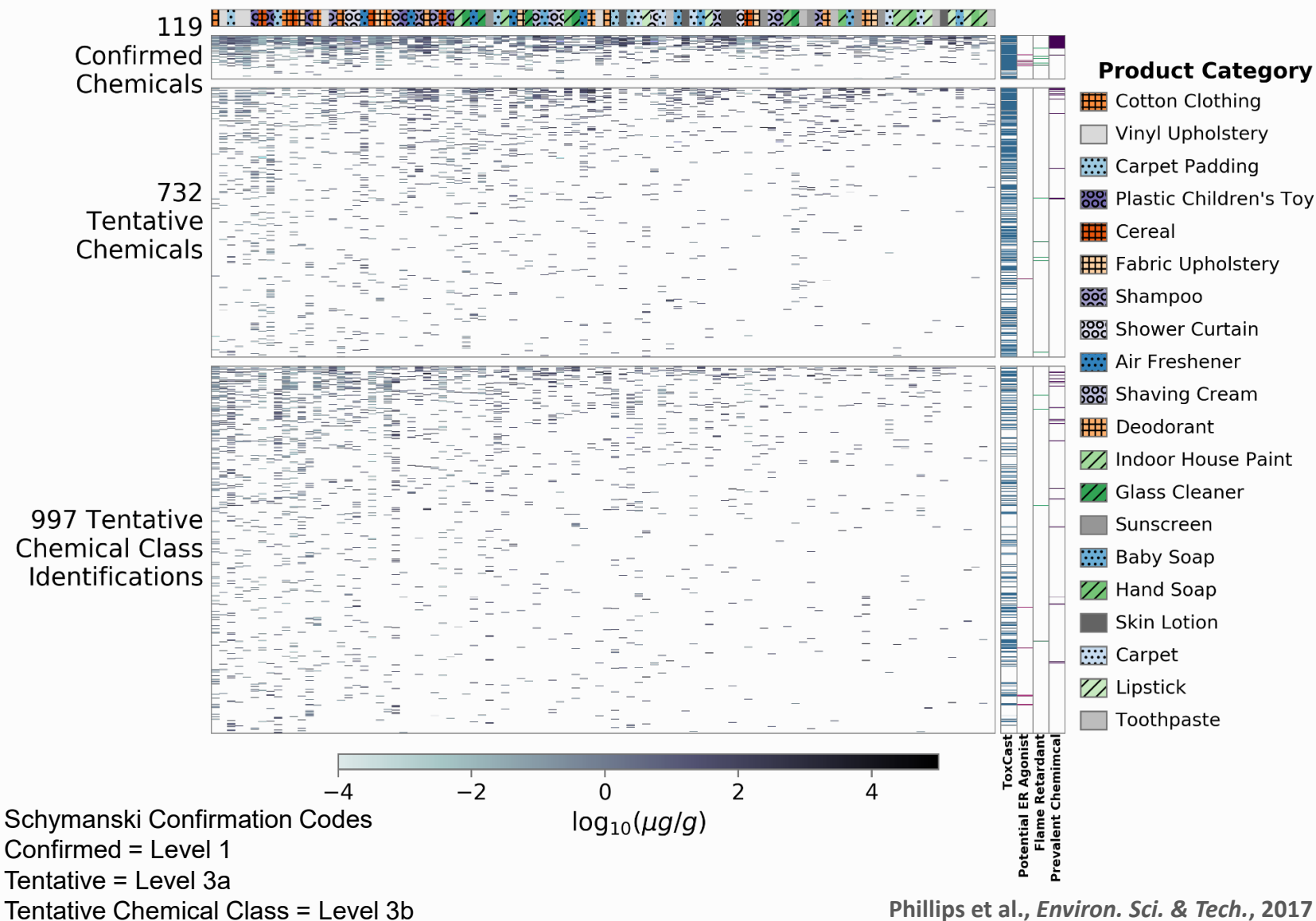


Access to CPDat



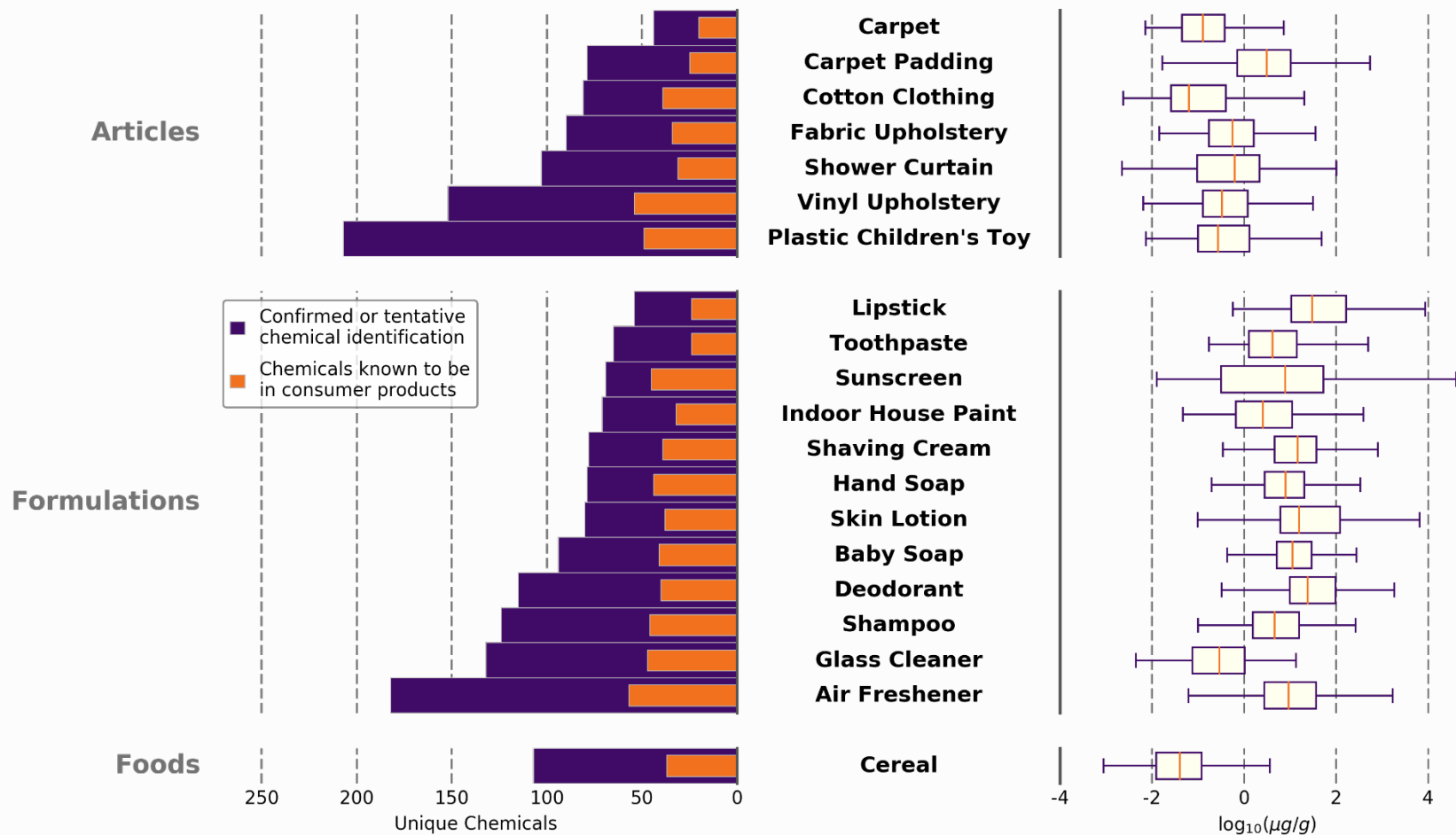
SSA Consumer Product Pilot Study

- Details:
 - GC × GC/TOF-MS
 - 100 Consumer Products across 20 product categories
- Only a small number of potential identifications get confirmed, the rest remain tentative identifications
- It is time consuming and expensive to get all standards for confirmation
- Challenge persists: How can we start to make sense of all the tentative identifications?



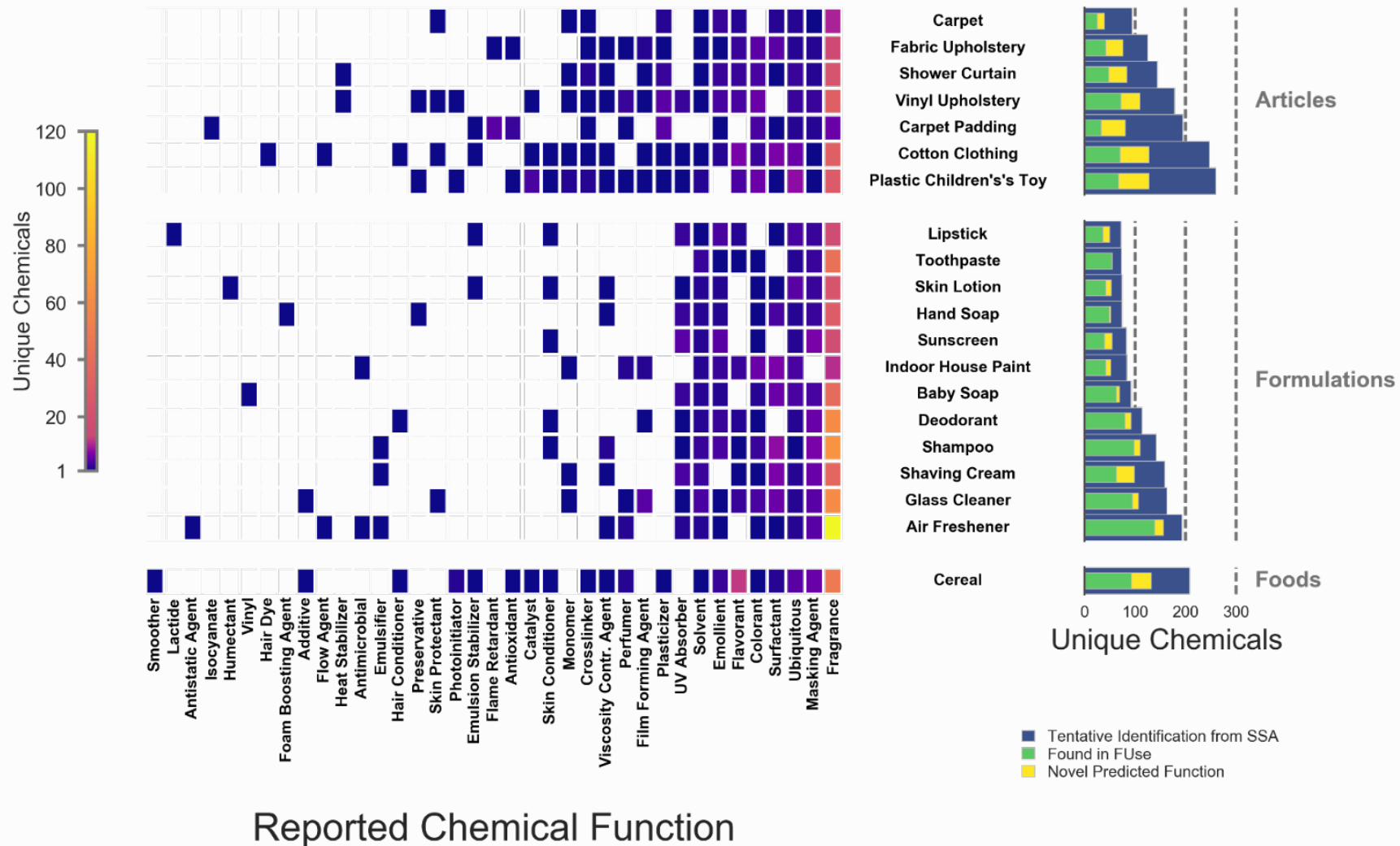
Comparing Identifications to Known Data

- SSA/NTA tells us we may have many compounds in these products
- CPDat tells us the compounds are not intentionally added to the products
- How do we tell which of these “unknown” chemicals should be there?



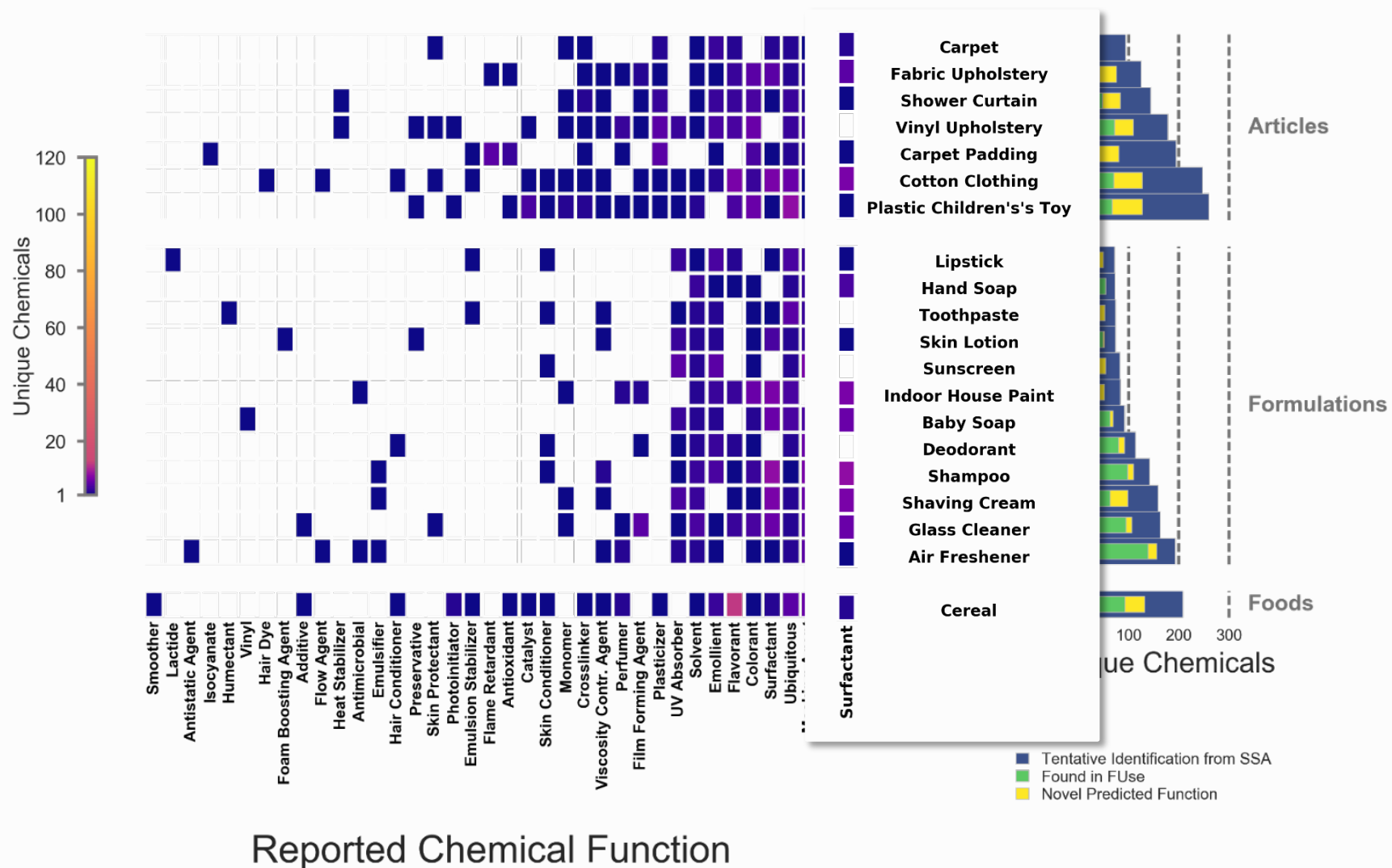
QSURs may help make sense of the rest

- Using functional use we can start to gather information on the tentative compounds
- Where there is no reported use, we can predict what a compound may be doing



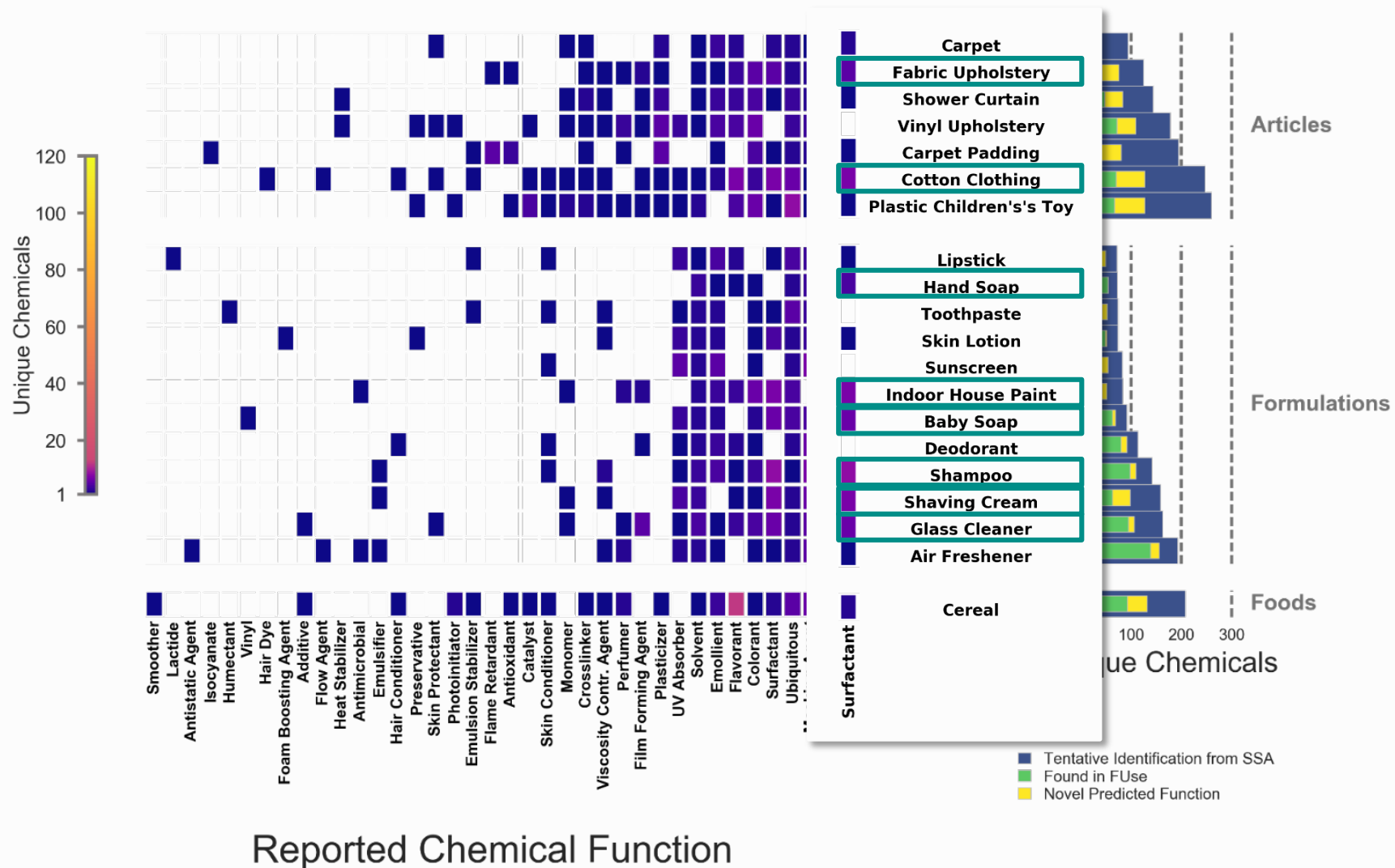
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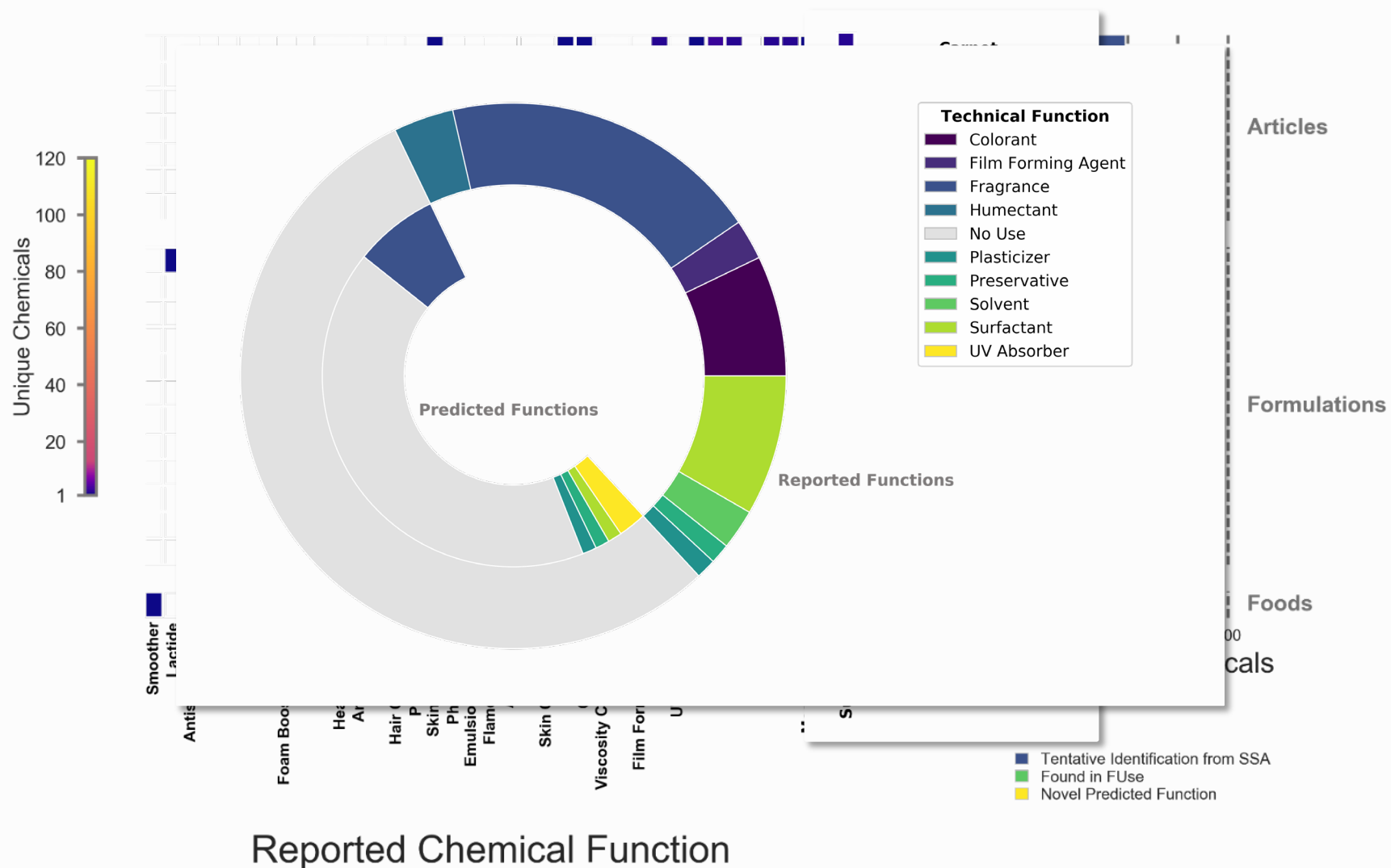
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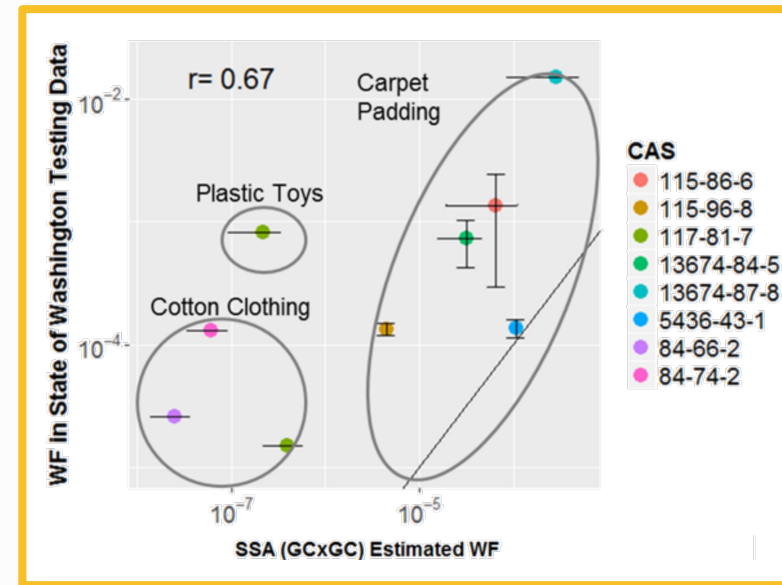
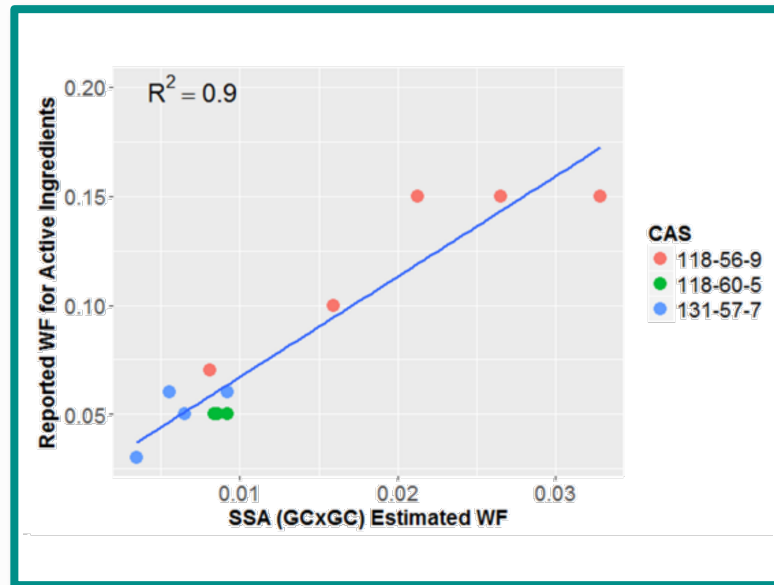
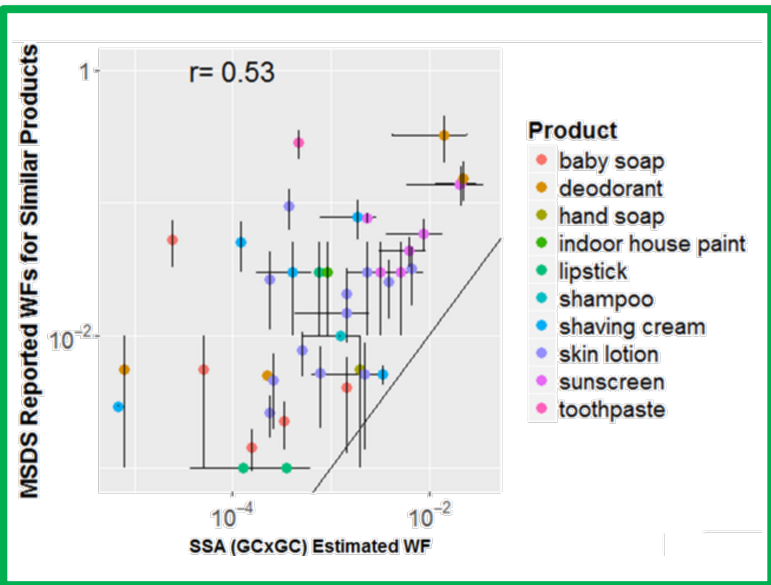


QSURs may help make sense of the rest

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CPDat Look-up of Chemical Concentrations



Material Safety Data Sheets:

- Manufacturer only required to report hazardous substances
- Reported over (typically) wide range of weight fractions
- 37 CASRN-product matches

Active Ingredients:

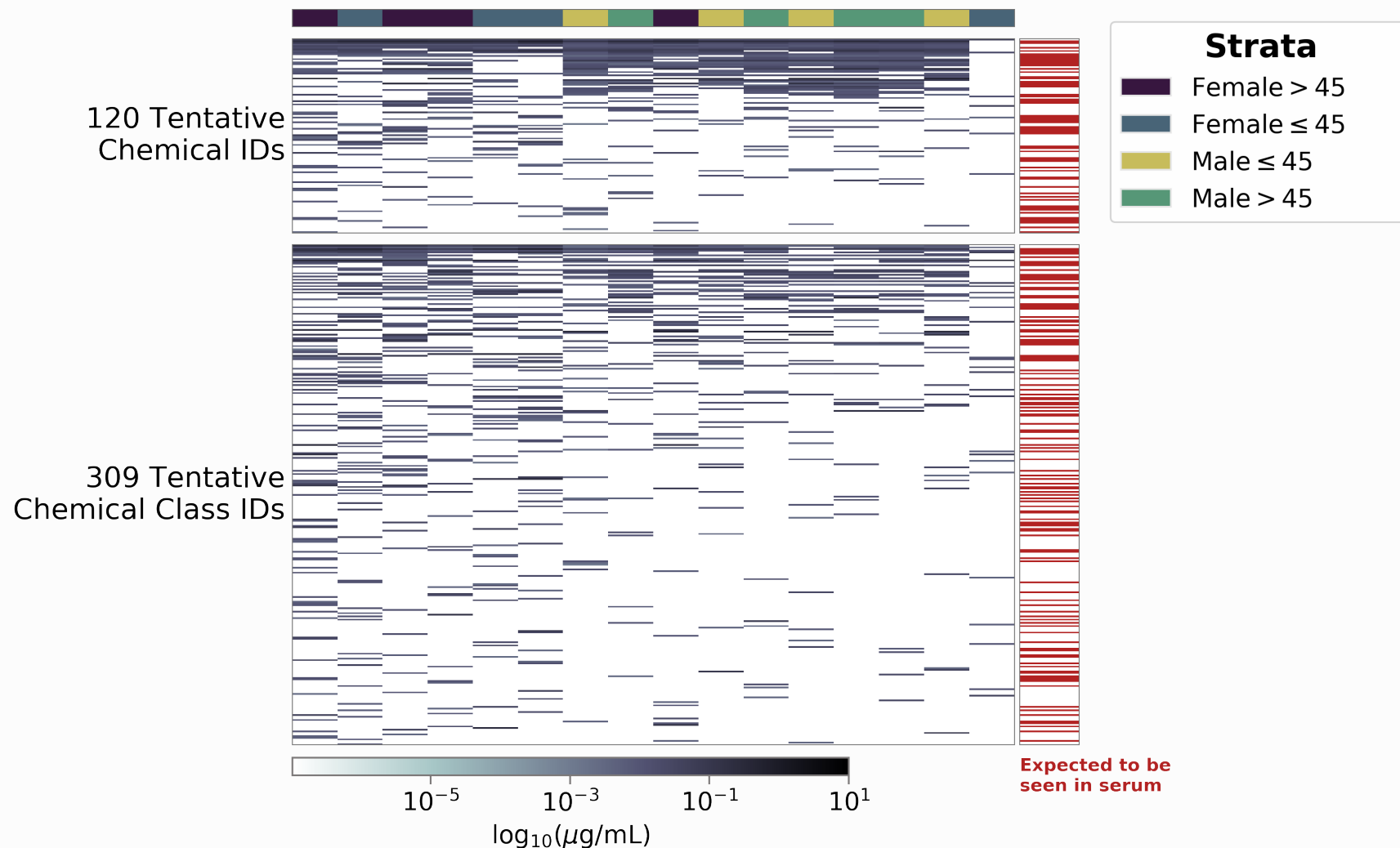
- FDA requirement to report known weight fraction
- All matches occurred in sunscreens
- 3 CASRN-product matches

State of Washington Product Testing Database:

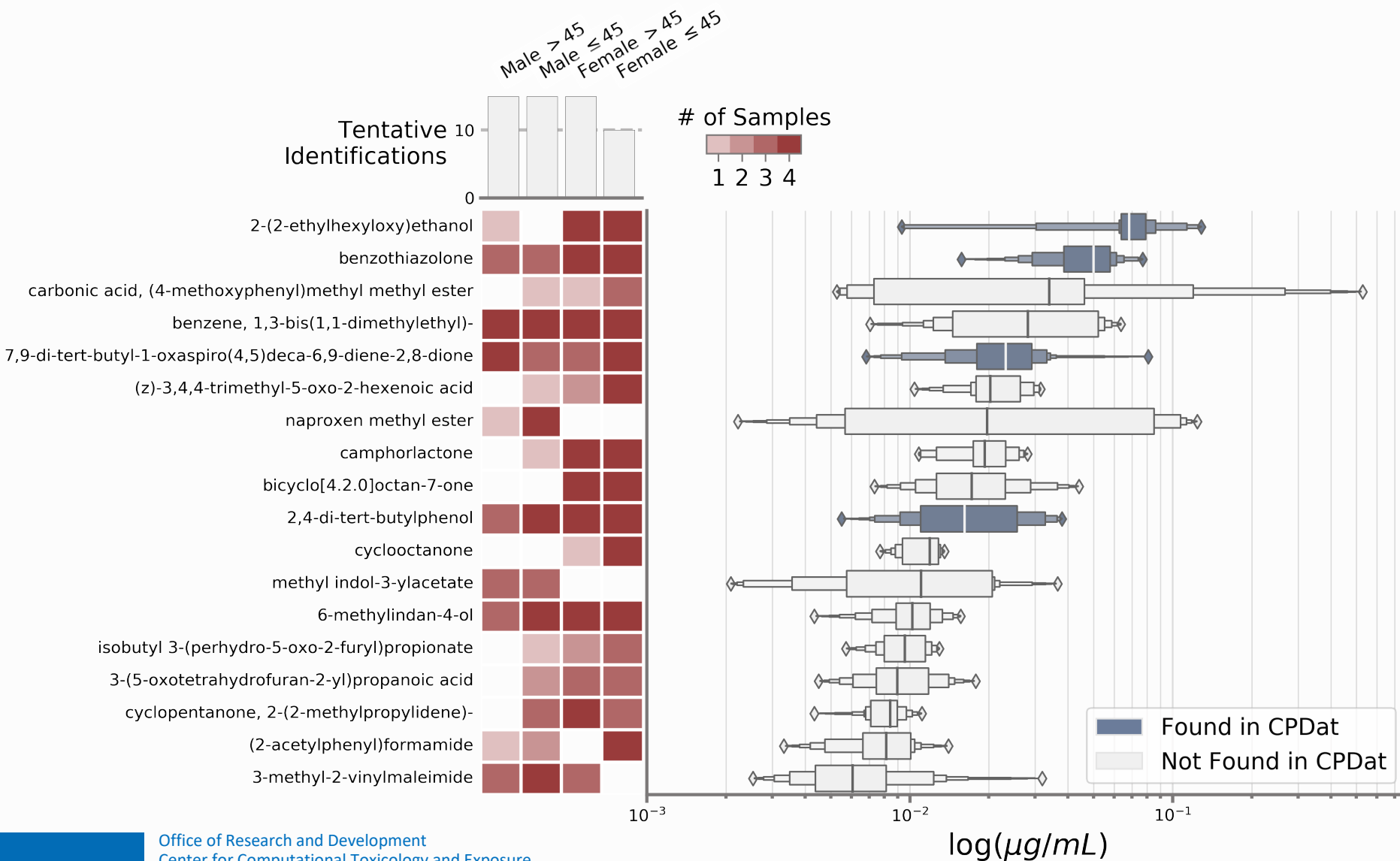
- Targeted analysis looking for specific chemicals
- 9 CASRN-product matches

Survey of the Data

- Details:
 - GC × GC/TOF-MS
 - 16 pooled blood samples from NIEHS
 - samples were 25 across individuals
 - 4 pooled samples exist for each strata
- Compounds expected to be in serum are either endogenous compounds or exogenous compounds that would be intentionally consumed (pharmaceuticals or food/nutrients)

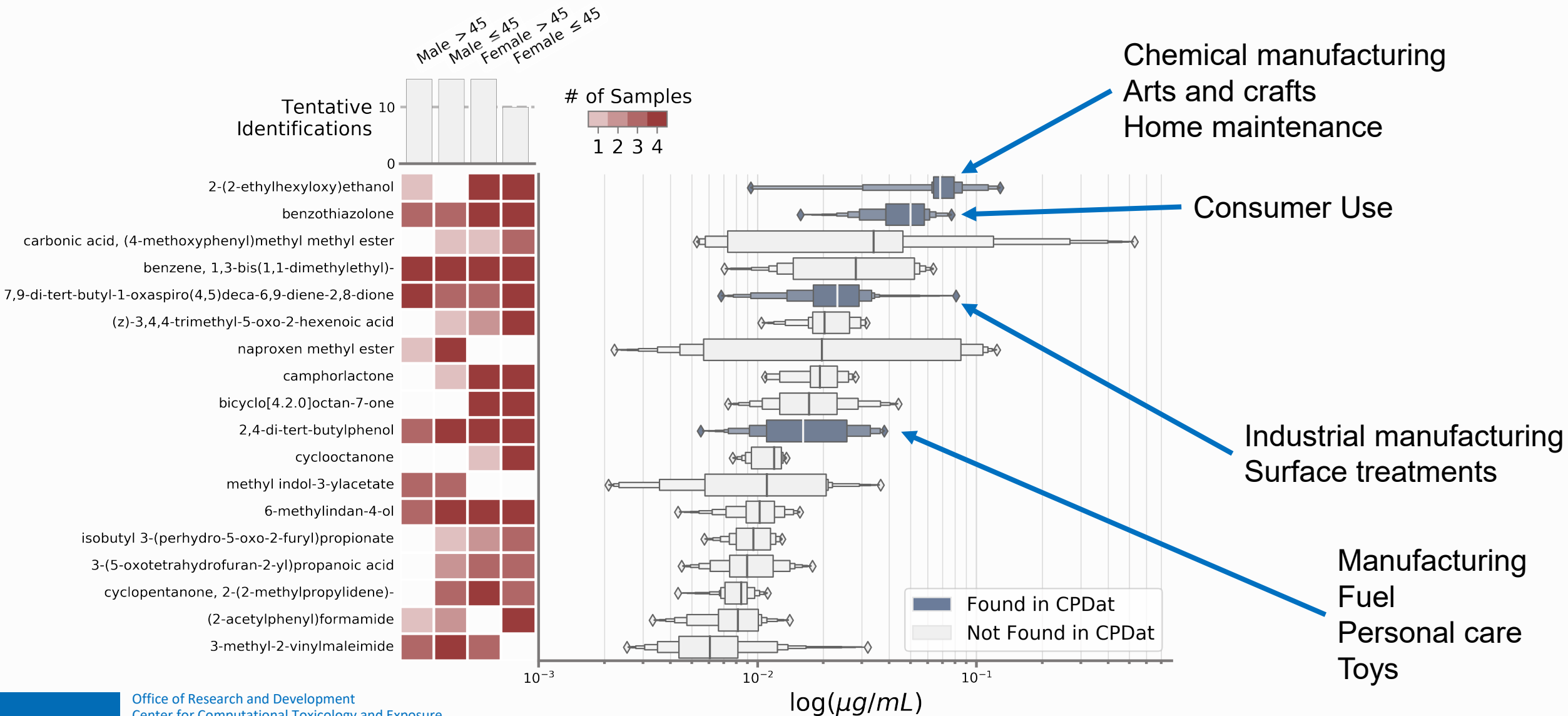


Commonly Occurring Chemicals

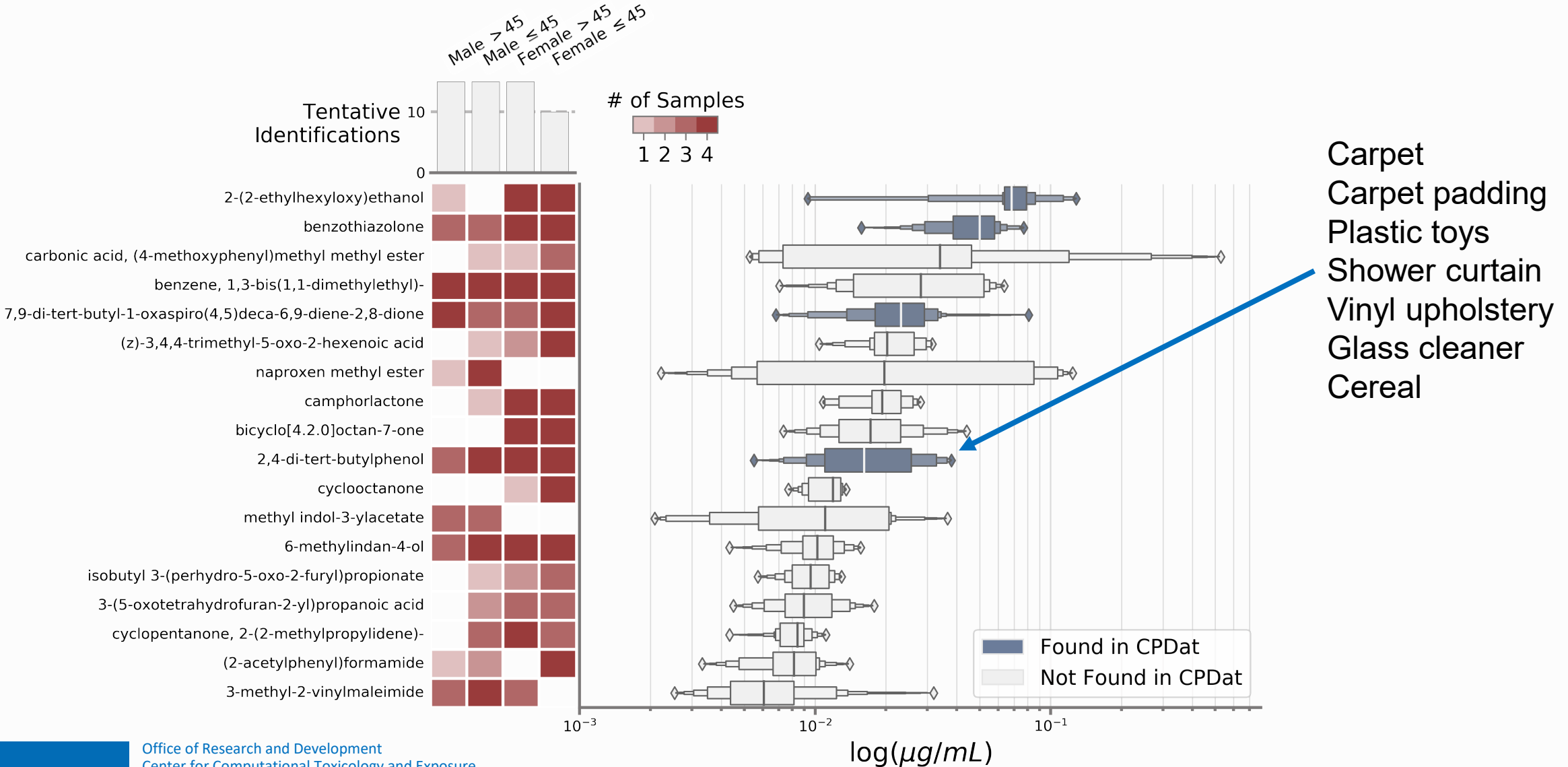


- Compounds that were not known pharmaceuticals, foods, or nutrients and were not endogenous
- Compounds that occurred in at least 4 of the 16 samples

Broad Chemical Categorizations



Tentatively Identified from Consumer Products SSA



Access to CPDat

