Potential Demographic Differences in Chemical Exposure Derived from Purchasing and Consumer Ingredient Data Streams

***Kristin K. Isaacs*, Zachary Stanfield, Kathie Dionisio, Rogelio Tornero-Velez, and Timothy Buckley**

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

Consumer Product Use and Exposure in Under-Represented Communities

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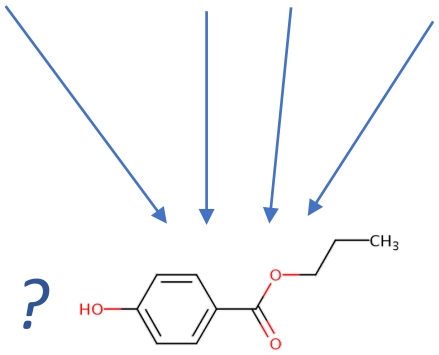
VIRTUAL EXPERIENCE

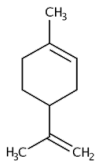
Introduction

- Empirical evidence from monitoring studies suggests that exposures vary by demographic
- Quantifying the impact of consumer exposure differences is complex
  - Humans encounter co-exposures to multiple chemicals
  - Behaviors (i.e., “habits and practices”) impact exposure and are driven by both needs and preferences
  - Monitoring studies target a limited set of chemicals
- In EPA’s Exposure Forecasting (ExpoCast) project, we are developing databases and tools that allow us to investigate consumer exposure to chemicals, including identification of chemicals with potential real-world co-exposures
- In addition to informing the selection of chemicals for testing in high-throughput screening, these approaches can elucidate demographic differences in exposures



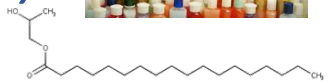
Roadmap

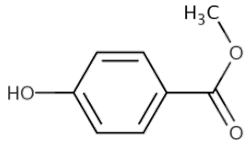
- Overview of an EPA effort to integrate available data related to consumer product purchasing behavior and consumer product chemical content
- Simple examples of drivers of potential exposure disparity
- Results from a holistic approach to examining co-exposures to chemicals, including potential endocrine disrupting chemicals

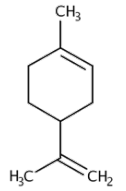


Behavior (Purchase and Use)

Chemical Content







Co-exposures?

Current Approach

- Integrate large datasets of consumer product ingredient and product purchasing information to develop a dataset that can be mined for information about exposure
- Purchase practices can be a surrogate for product use patterns
- Apply informatics approaches (frequent itemset mining) to quantify differences in product purchasing and related introduction of chemicals into households
- Stratified results by household demographics to characterize variability in co-exposure patterns and identify potential chemical combinations associated with sensitive populations, such as families with young children, women of childbearing age, or households led by women of color

Purchasing Data

Chemicals and Products Database (CPDat)

Ingredient Data

Products and Chemicals introduced to Household

{Product A, Product B, Product C…}

{Chemical 1, Chemical 2, Chemical 3, Chemical 4, Chemical 5…}

Differences in Habits and Practices
Prevalent Potential Co-Exposures

EPA-ORD's Chemicals and Products Database (CPDat)

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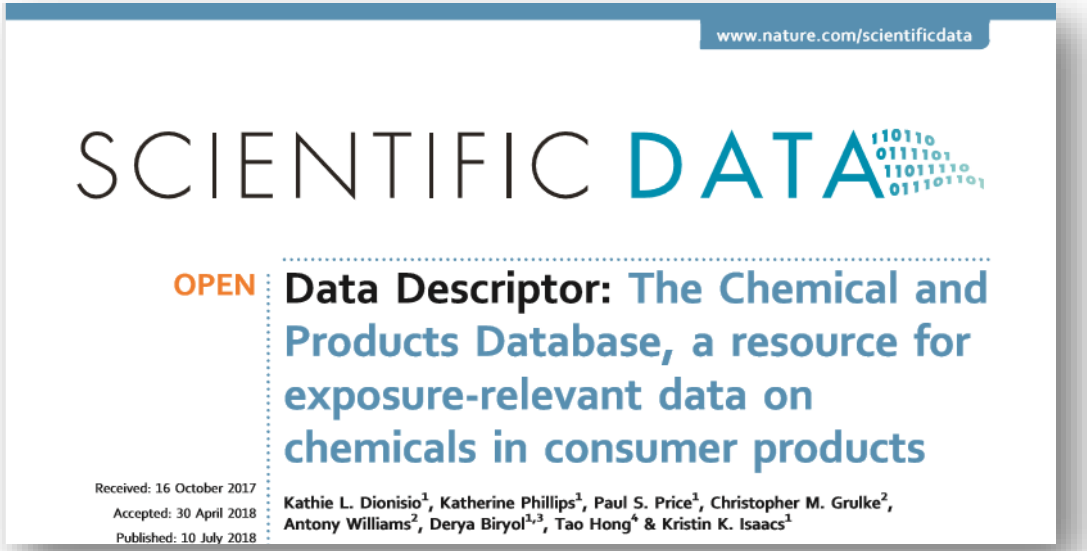
- EPA ORD database containing curated chemical use and consumer product ingredient data
- Public version of the dataset contains ingredient data for over 60,000 products, mapped to standardized product categories for use in exposure assessment and modeling
- Also recently extracted ingredient data from 230,407 retailer-provided product safety data sheets (SDSs), including product name, category, universal product code (UPC), and chemical identifiers
- Chemical identifiers were mapped to unique DTXSIDs (identifiers used by the EPA CompTox Chemicals Dashboard).


www.nature.com/scientificdata

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]

Dionisio et al. Sci Data 5:180125 (2018).

https://www.epa.gov/chemical-research/chemical-and-products-database-cpdat

https://comptox.epa.gov/dashboard

Consumer Product Purchasing Study

- EPA initiated a collaboration with Nielsen in 2013
- Shared data from the National Consumer Panel (NCP)
- Formerly called “Homescan” project

Nielsen Purchasing Data

- 60,000 U.S. households for 1 year (2012)
- Demographic information for each household
  - Income, number of household members, Nielsen market (metro area), county size, race, presence and age of children, age and occupation of female head of household
- All purchases for product categories of interest to Nielsen
  - 29 broad categories called “Groups” (e.g., Household Cleaners, Cosmetics, Fresheners and Deodorizers).
  - Date of purchase, UPC, brand, number of units, size
  - ~4.6 million individual product purchase records
- 133,966 unique product UPCs
- Recent publication: Tornero-Velez et. al (2020) examined product co-purchases which gave us some idea about chemical co-exposure from previous ingredient data; the ability to link individual purchases to specific chemicals is a major step forward.

Tornero-Velez et al., Risk Analysis, 125:8, 2017

Data Integration and Frequent Itemset Mining

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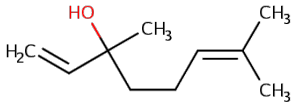
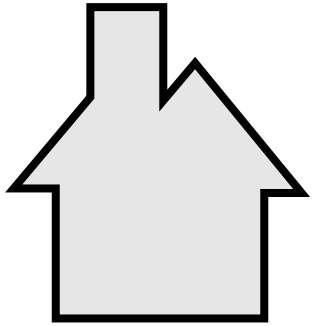
Products Purchased By the Household from Nielsen Survey



CPDat
Chemical and Products Database

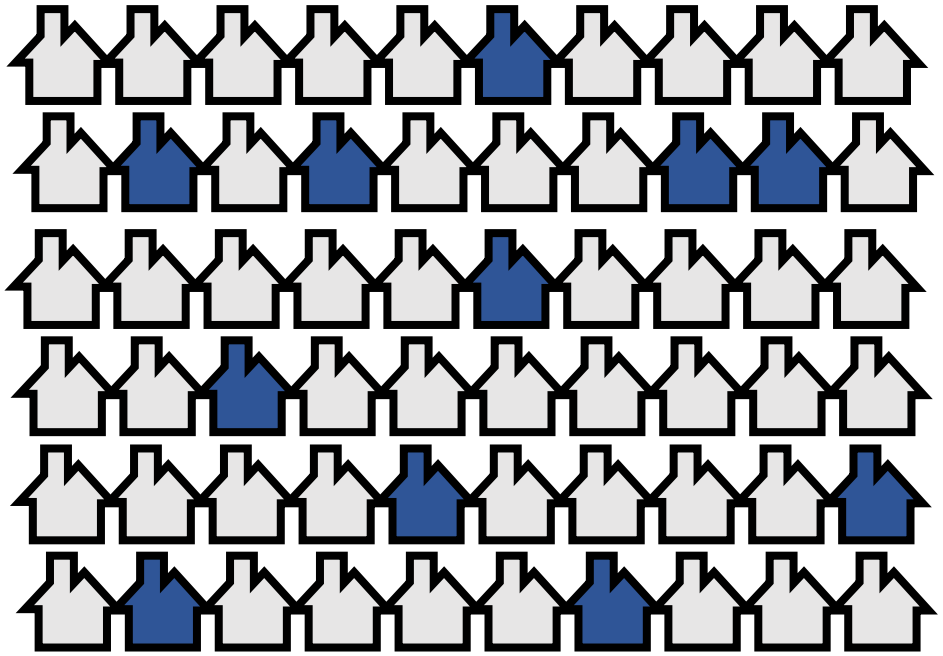
Chemical Ingredients of Products



{Chemical1, Chemical2…..Chemical 50}

Chemicals Introduced to Each Household Through Product Purchases

60,000 Households



Frequent Itemset Mining
Combinations > Threshold % households

{Chemical1, Chemical8, Chemical 20}

Prevalent Chemical Combinations

Chemical Lists Evaluated

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- Analysis was restricted to chemicals of regulatory or biological interest in order to avoid identification of prevalent chemical combinations containing common substances having little relevance to risk assessment (e.g., water)
- **Broad Chemical List:** Active public chemical inventory of the Toxic Substances Control Act (TSCA)
  - **649** chemicals in the consumer product transaction dataset
- **Case-Study: Potential Endocrine Active Chemicals (EACs)**

Source	Investigated Biological Action	Chemicals Predicted to be Active	Chemicals Mapped to Purchased Products
Collaborative Estrogen Receptor Activity Prediction Project (CERAPP)[1]	Estrogen Disruptors	1,142	10
Collaborative Modeling Project for Androgen Receptor Activity (COMPARA)[2]	Androgen Disruptors	16,112	42
Additional potential EACs from Literature Sources[3]	Multiple		17
Total (unique)			**65**

[1]*Mansouri, K. et al. 2016. Environmental Health Perspectives. 124:1023-1033.*
[2]*Mansouri, K. et al. 2020. Environmental health perspectives. 128:27002.*
[3]*Dodson et. al. Environmental health perspectives. 120:935-943.*

Example Simple Comparison: Race, Product Type, and Brand Choice

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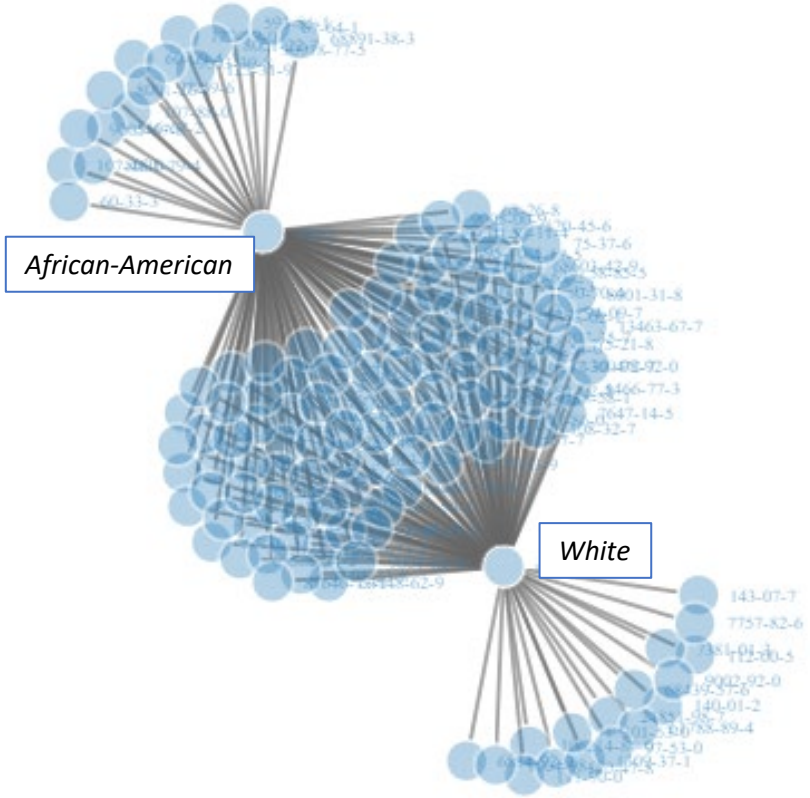
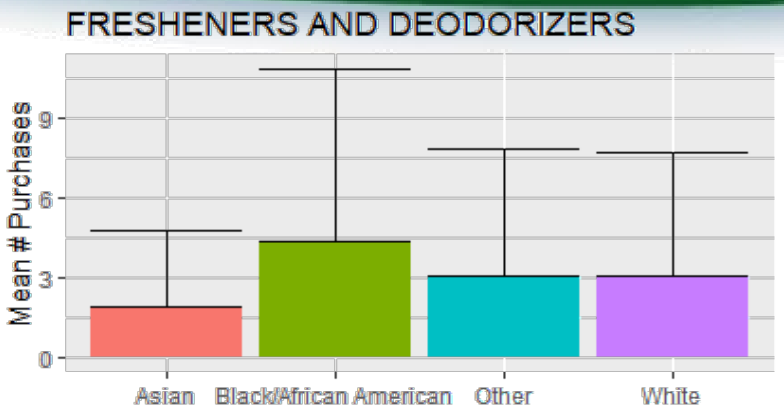
The chemicals to which people are exposed have the potential to be influenced by the types of products purchased and potentially brand choice.

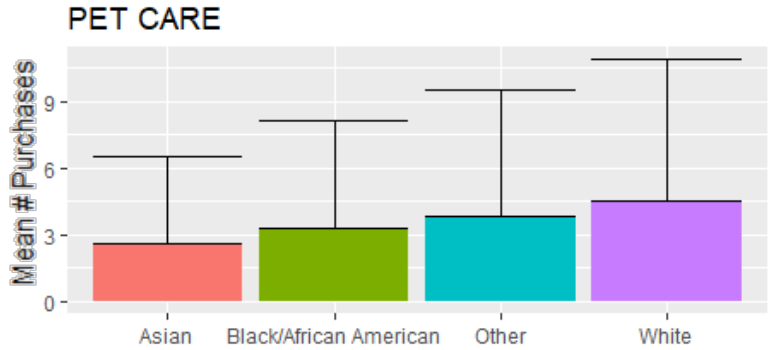


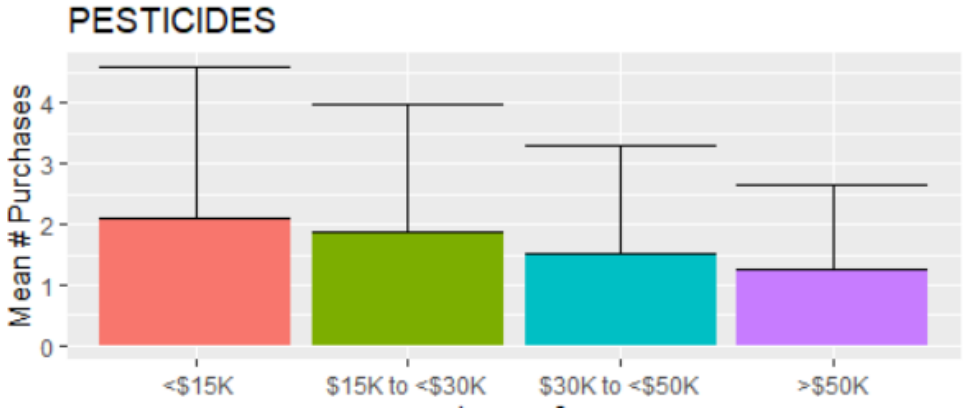
Hair Styling Products

- Universe of 100+ unique chemicals matched to "Hair Care Preparations" (styling products)
  - Caveat: recall incomplete matching and some bias towards White middle class households
- There were sets of chemicals unique to both White and African American (AA) households
- Chemicals unique to AA households were primarily associated with products/brands marketed (primarily) to AA populations (pressing oils, growth oils, strengtheners, relaxers)
  - Acetone in a pressing oil
  - Polyvinylpyrrolidone in hair growth oil
- Chemicals unique to White households were from various products, many from "specialty" brands
  - Dodecyltrimethylammonium chloride in texturizing cream
  - Eugenol (fragrance) in a defrizzing serum

Examples of Differences in Purchasing Patterns







- Many differences ***in number of purchases per person*** across demographics (e.g., race and income) for various product families
- Significant differences in ***ounces/person purchased*** by the household in a year across demographic variables (Kruskal-Wallis test)
  - Female Head Age: **107** product types
  - Race: **97** product types
  - U.S. Census County Size: **63** product types
  - Number/Age of Children: **81** product types
  - Hispanic/Non-Hispanic: **51** product types
  - Income: **67** product types
  - Female Head Occupation: **60** product types
- Moving forward: Can we identify key "consumer household types" based on habits and practices, rather than looking at explicitly pre-defined groups? Might that address exposure in a meaningful way by capturing interactions?
- What do these differences mean in terms of chemical exposure?

Chemical Combination Results: Orientation

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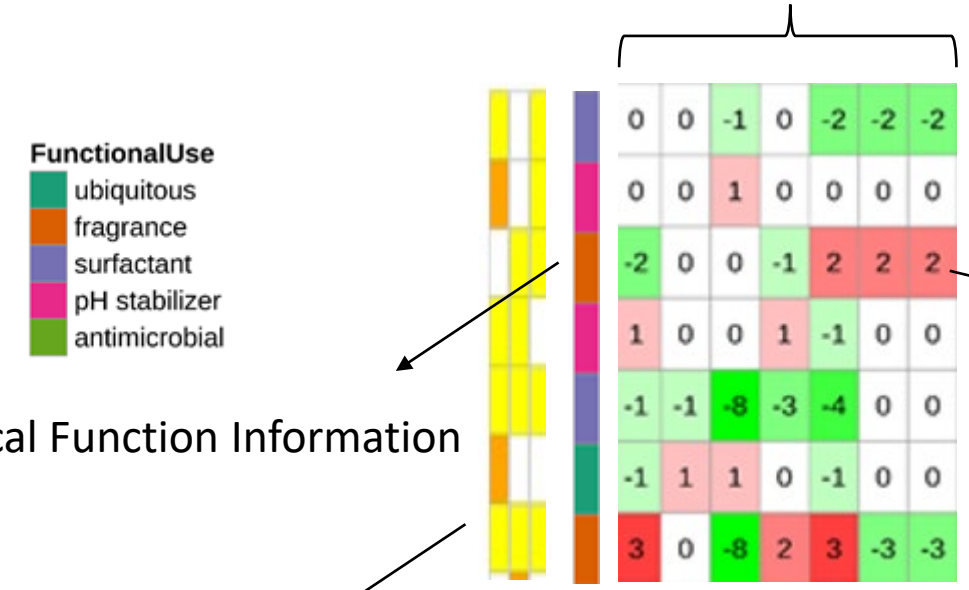
Demographic



{Chemical or Chemical Combination}

Chemical Function Information

Receptor Information

Deviation of the *rank* of the chemical or combination for each demographic from the rank in the population overall

Elevated rank relative to overall population
Potentially higher exposure for the demographic

Reduced rank relative to overall population
Potentially lower exposure for the demographic

Most Prevalent Single Chemicals

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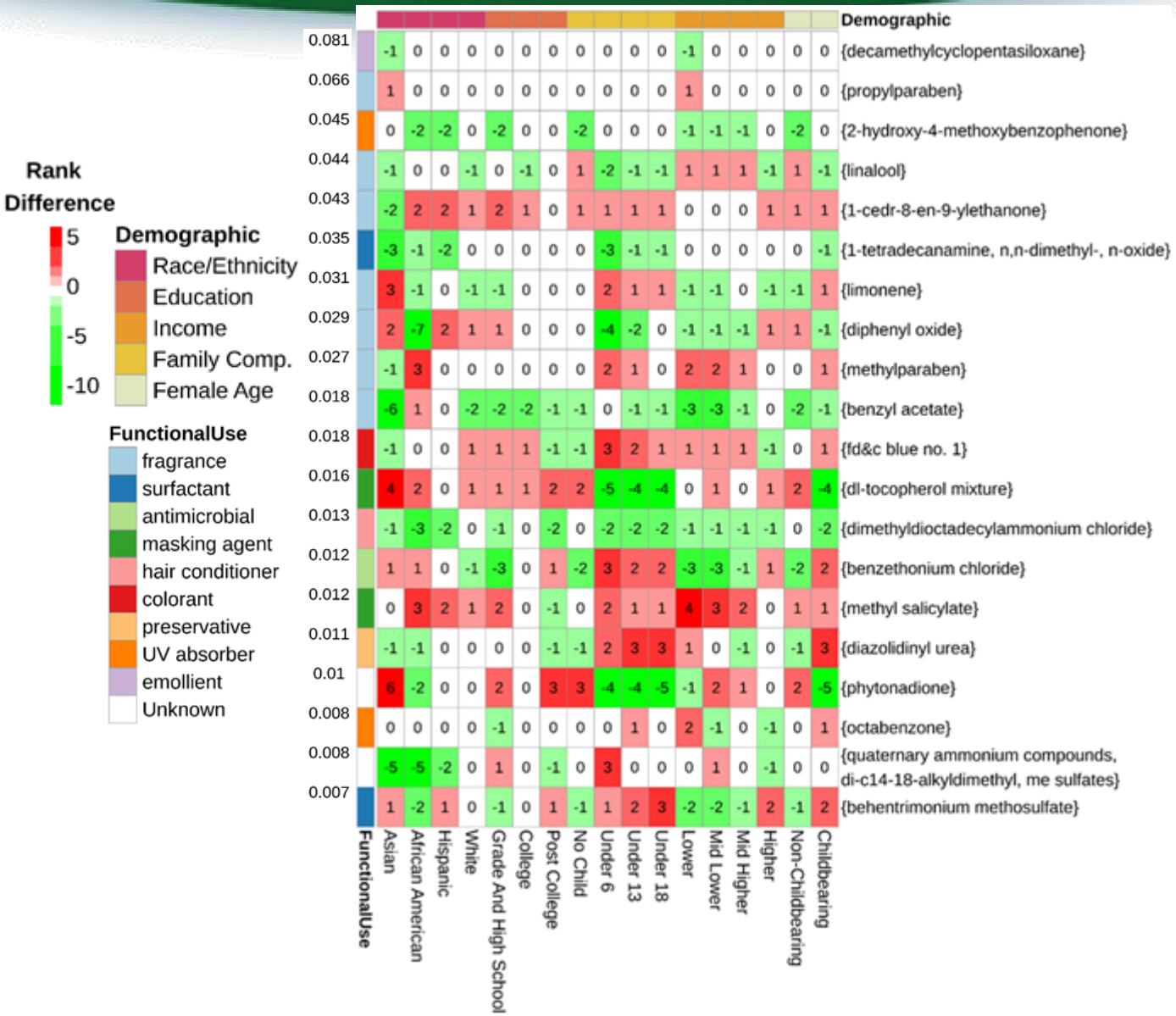


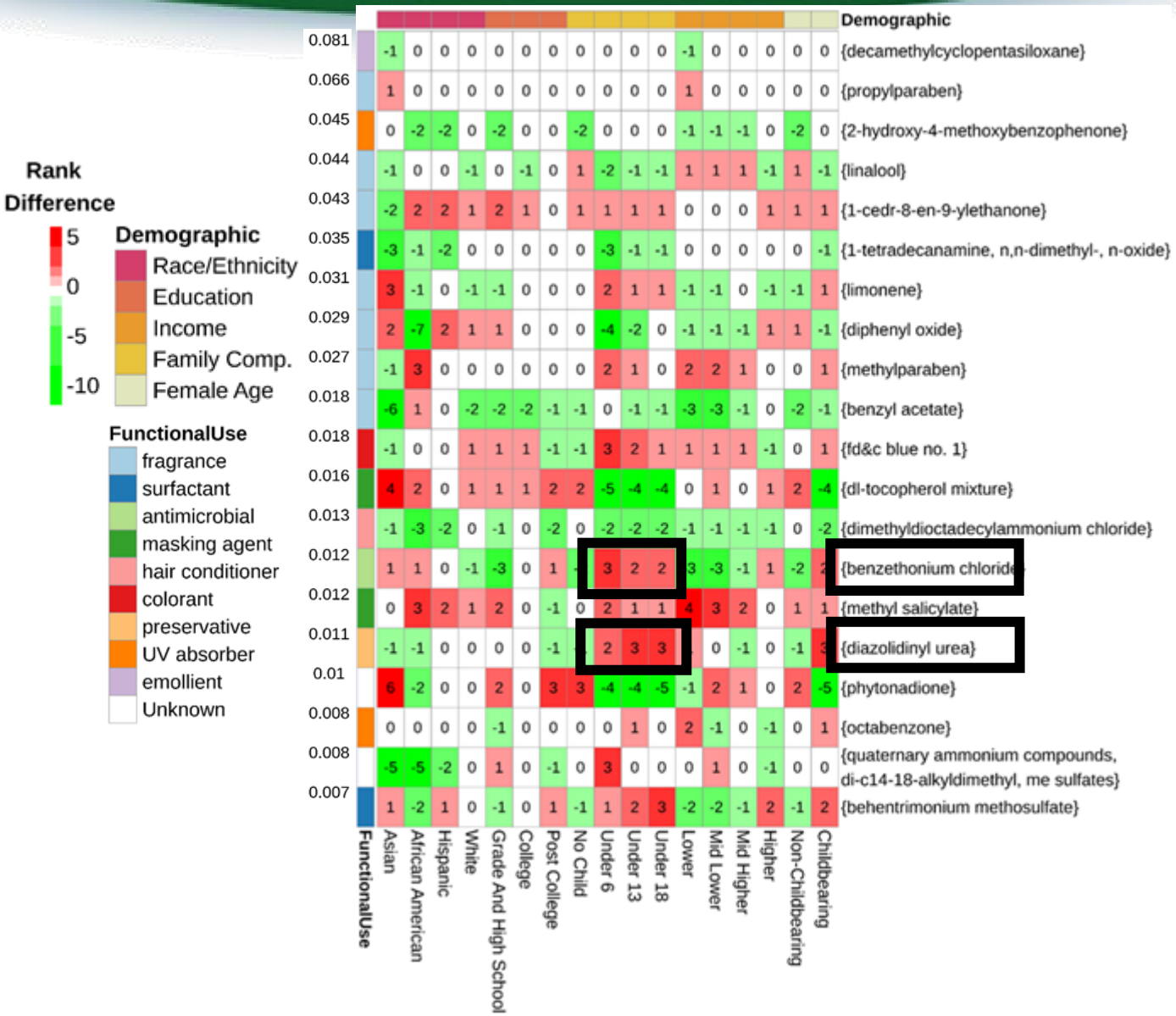
Endocrine Active Chemicals

- Many of the most prevalent EAC chemicals were fragrances (or categorized as such due to presence in fragrance formulations)
- Many of these chemicals were present in a variety of personal care products

Stanfield et al. EHP, 2021

Most Prevalent Single Chemicals

United States Environmental Protection Agency



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- *Benzethonium chloride* and *diazolidinyl urea*, which were ranked 2 or 3 places higher in households with children, are commonly used as topical antimicrobial agents in baby wipes, bubble baths, cosmetics, and skin care products

Stanfield et al. EHP, 2021

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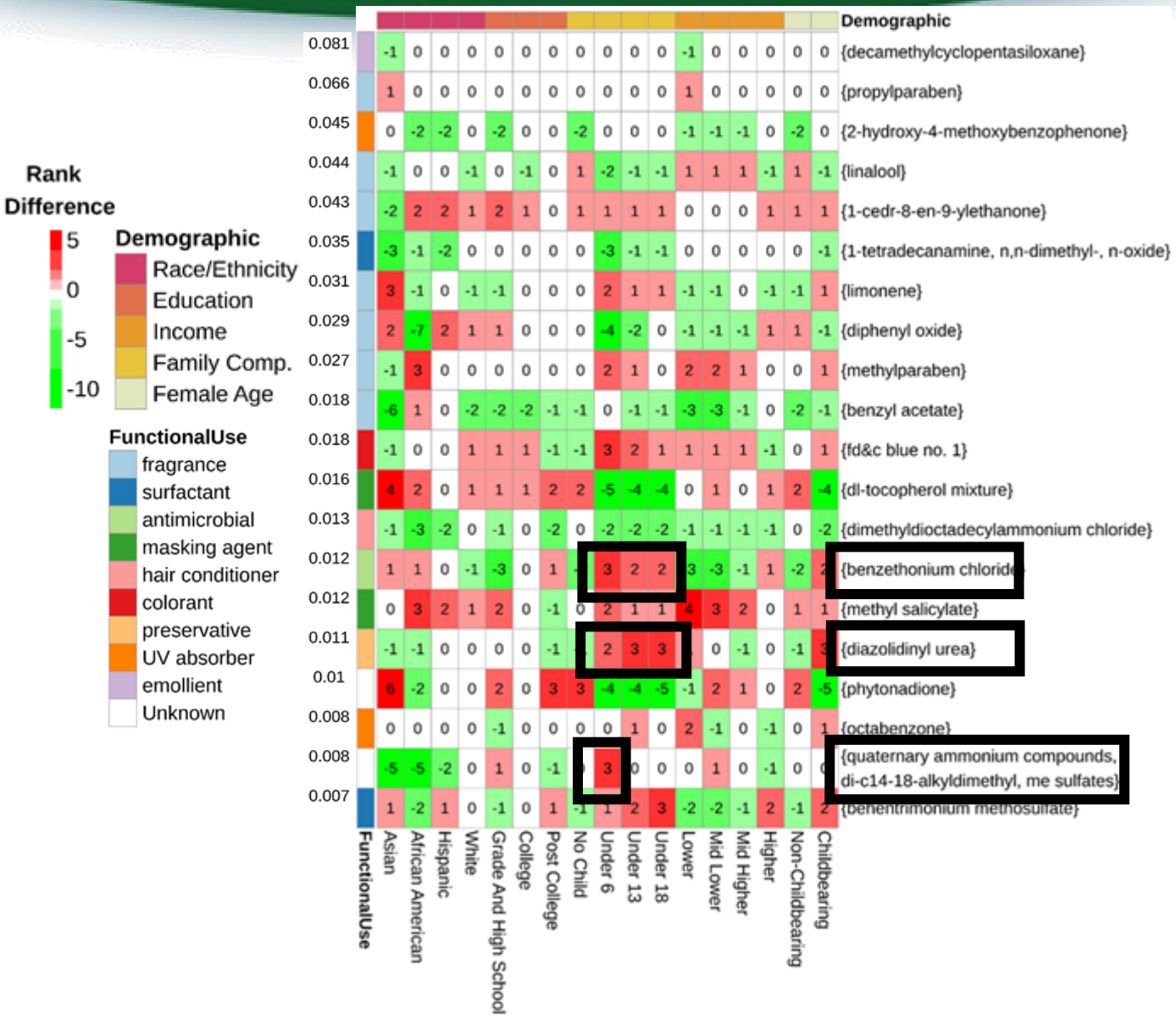

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- Households with children under 6 have a higher ranking for *quaternary ammonium compounds, di-c14-18-alkyldimethyl, me sulfates*, which are commonly used in disinfectants and hand soaps

Stanfield et al. EHP, 2021

Prevalent Combinations

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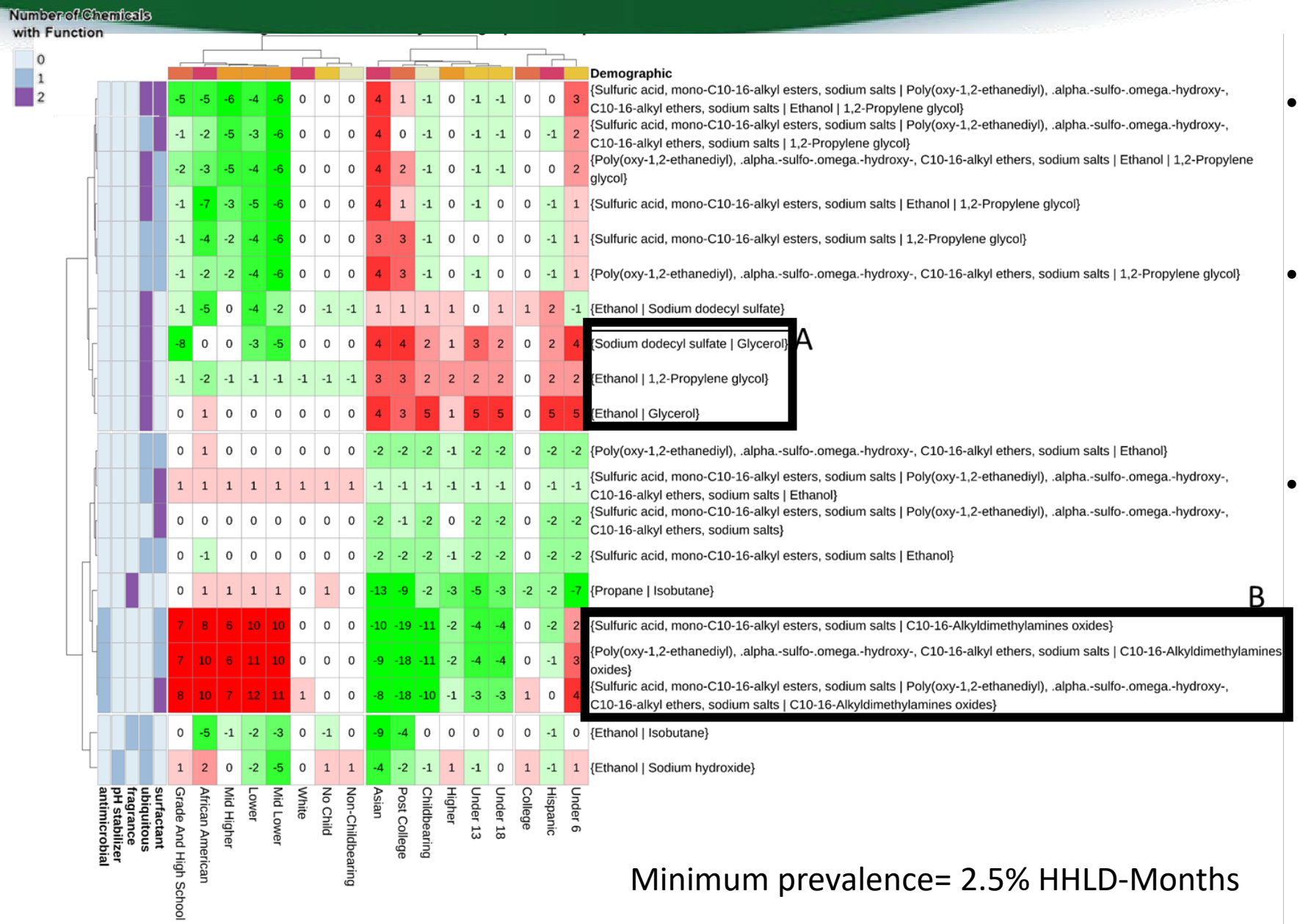


Minimum prevalence= 2.5% HHLD-Months

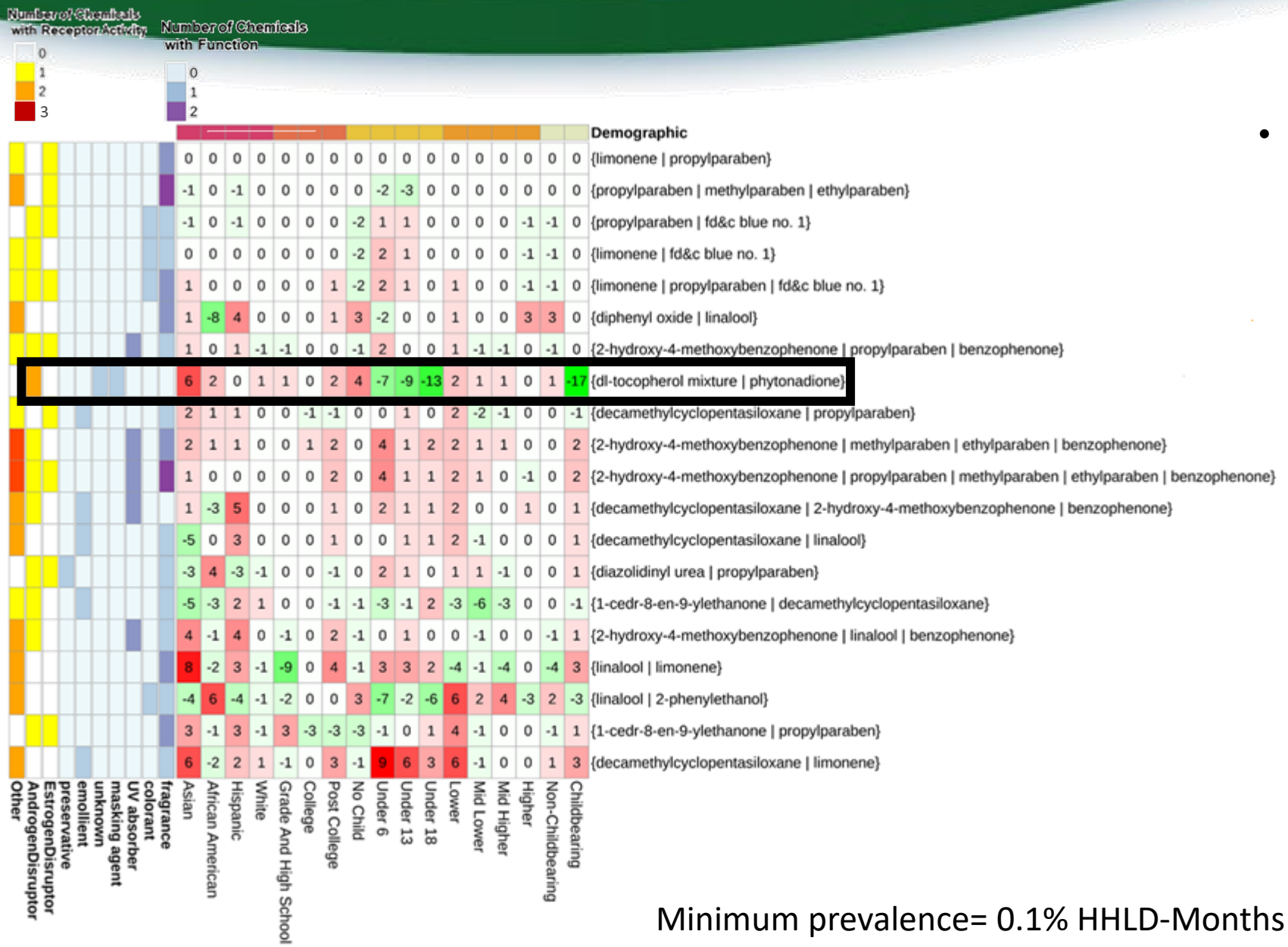
Group 1 (Broad TSCA Inventory)

- Here demographics and chemical sets are clustered to indicate the similarity of rankings of chemical combinations
- Set A: ubiquitous consumer product chemicals present in households with children, higher income, and more highly educated, representing generally high consumer product use
- Set B: elevated difference in rank in lower to middle income demographics and African American households, and reduced rank differences in Asian households and females with post-college education and females of childbearing age; these three sets contained antimicrobials and surfactants found in cleaning products

Stanfield et al. EHP, 2021

Prevalent Combinations

United States Environmental Protection Agency



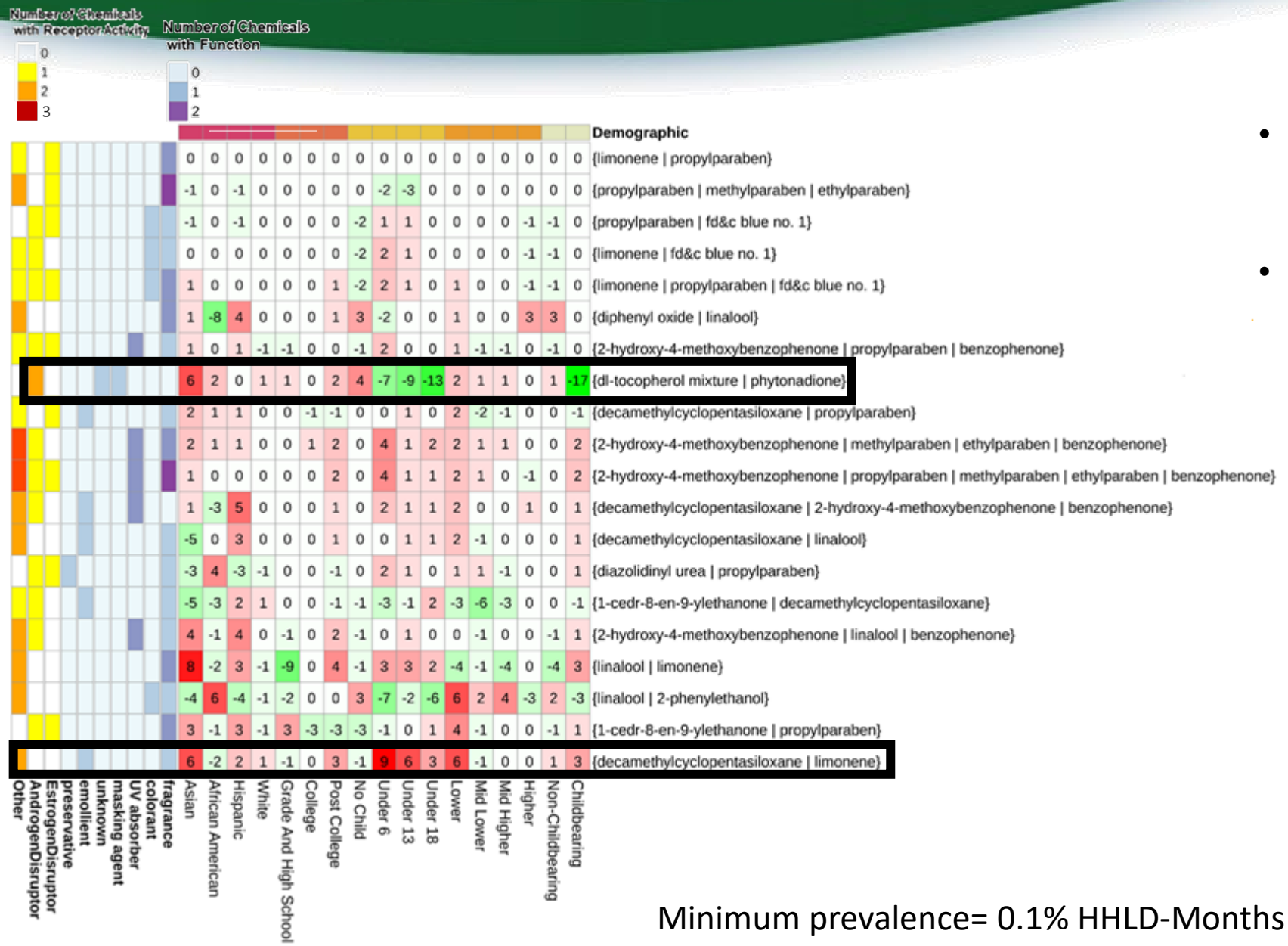
Endocrine Active Chemicals

- One itemset {*dl-tocopherol mixture* | *phytonadione*}, contained two chemicals that targeted the same receptor (AR).

Minimum prevalence= 0.1% HHLD-Months

Stanfield et al. EHP, 2021

Prevalent Combinations



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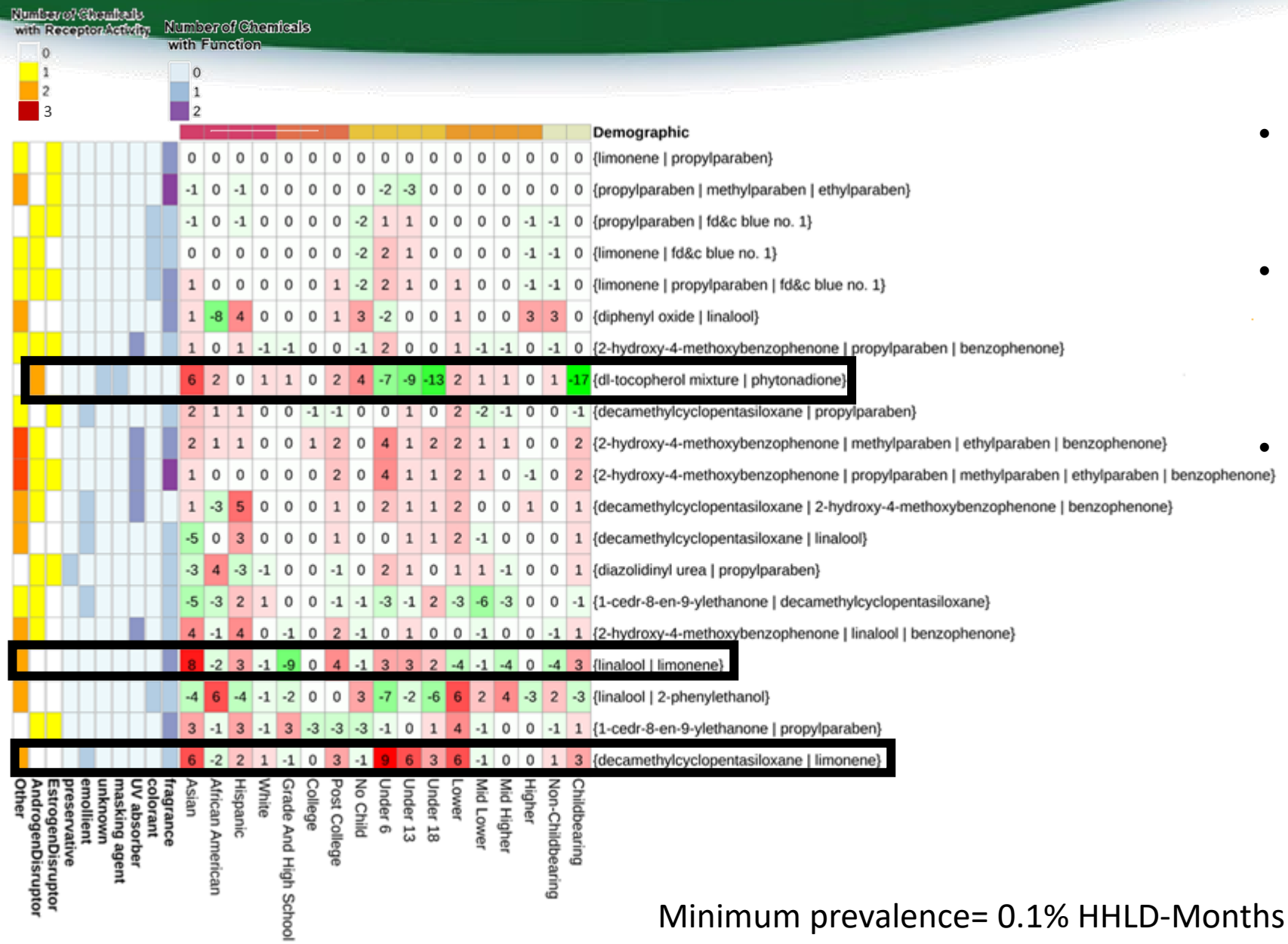
Stanfield et al. EHP, 2021

Prevalent Combinations



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- Households with a female head of Asian race had the highest positive rank departure for the combination of *limonene* and *linalool*, the latter of which is used as a scent in many perfumed hygiene products and cleaning agents.

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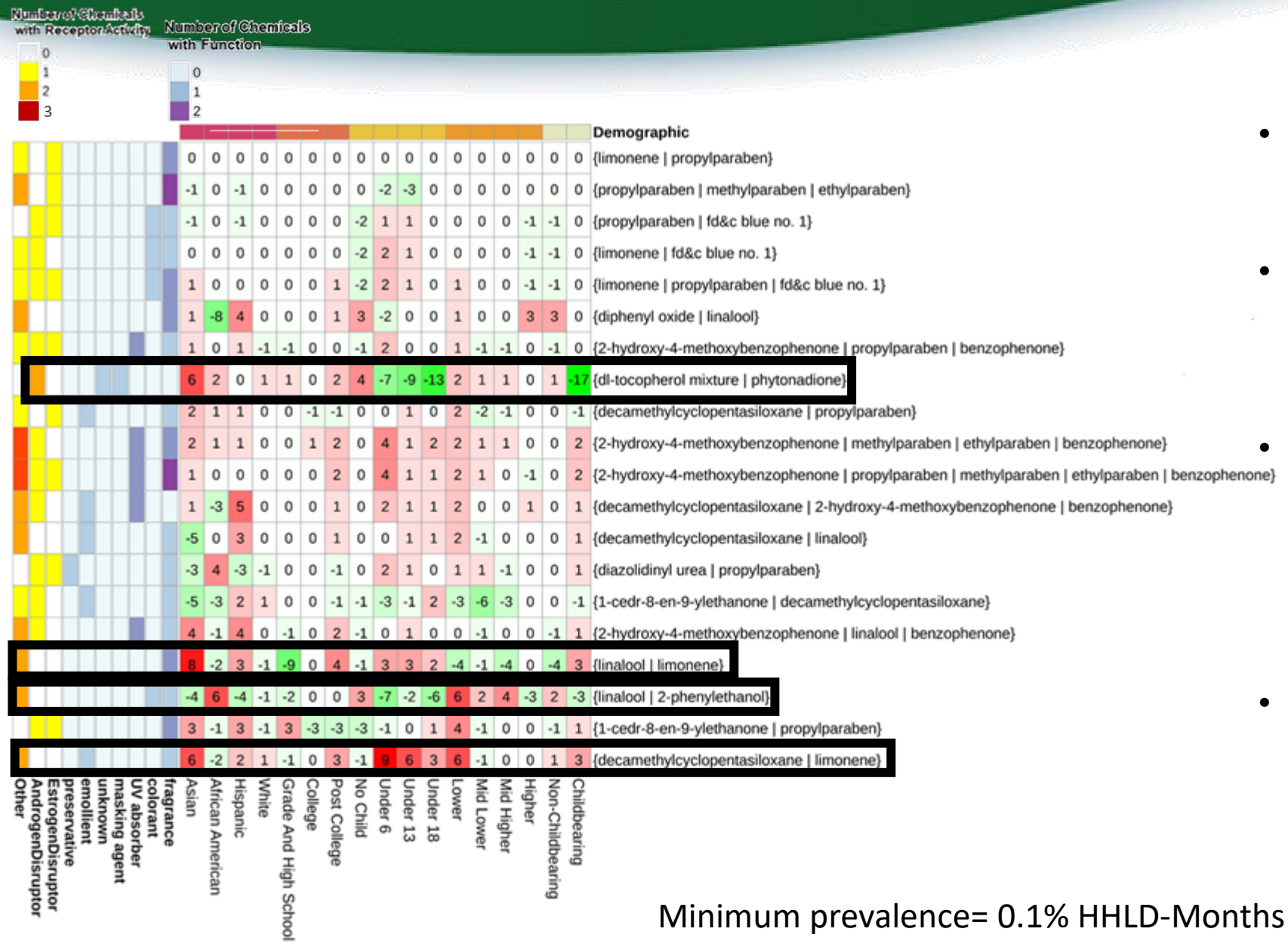

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- African American households had a positive rank departure of 6 for the combination {*linalool* | *2-phenylethanol*}; the second chemical is a floral fragrance primarily present in air fresheners.

Stanfield et al. EHP, 2021

Summary and Future Work

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- Collectively across all products and by product group, results indicated that households with children, households headed by women of color, and lower income households exhibited divergence from the general population in the chemical combinations they encounter most frequently.
  - This may be due to a need for different types of personal care products designed specifically for given races or ethnicities, brand or regional preferences, or simply the need for a wider variety of products in households with multiple children.
  - These patterns reflect differential experiences and thus differential exposures among demographics.
- New non-targeted analysis (NTA) studies of biological media such as blood or urine can complement and evaluate predictions of co-exposures associated with consumer products.
  - Such studies also have the potential for identifying mixtures containing metabolites of consumer product chemicals.
- These results can inform toxicity testing of real-world chemical combinations, as well as design of monitoring studies, including consideration of sensitive or under-represented groups.

Project Team

Cody Addington
Timothy Buckley
Kathie Dionisio
Kristin Isaacs
David Lyons
Katherine Phillips
Zachary Stanfield
Rogelio Tornero-Velez

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