We are Living in a Material World: Indoor Chemistry and Exposures

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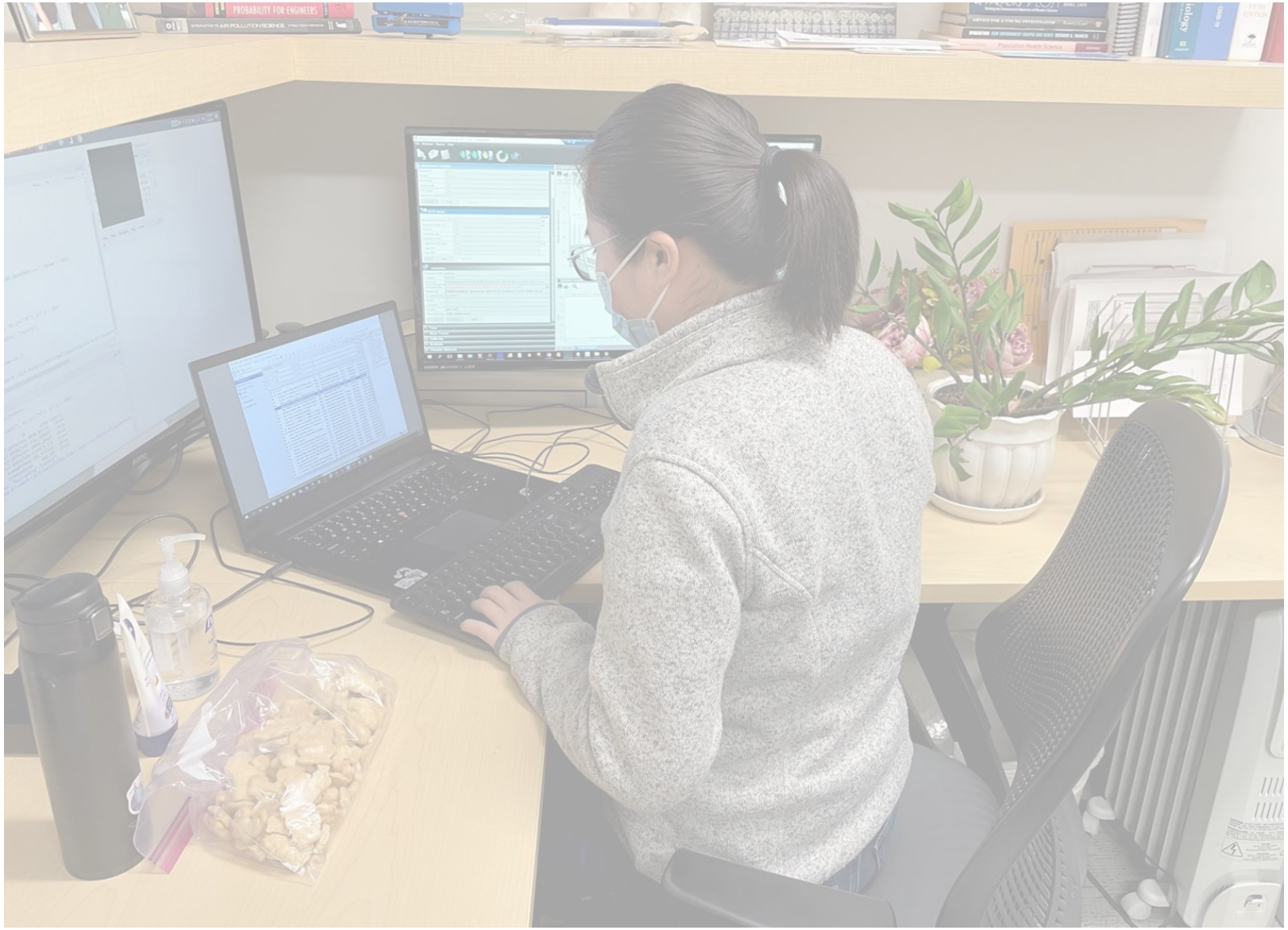
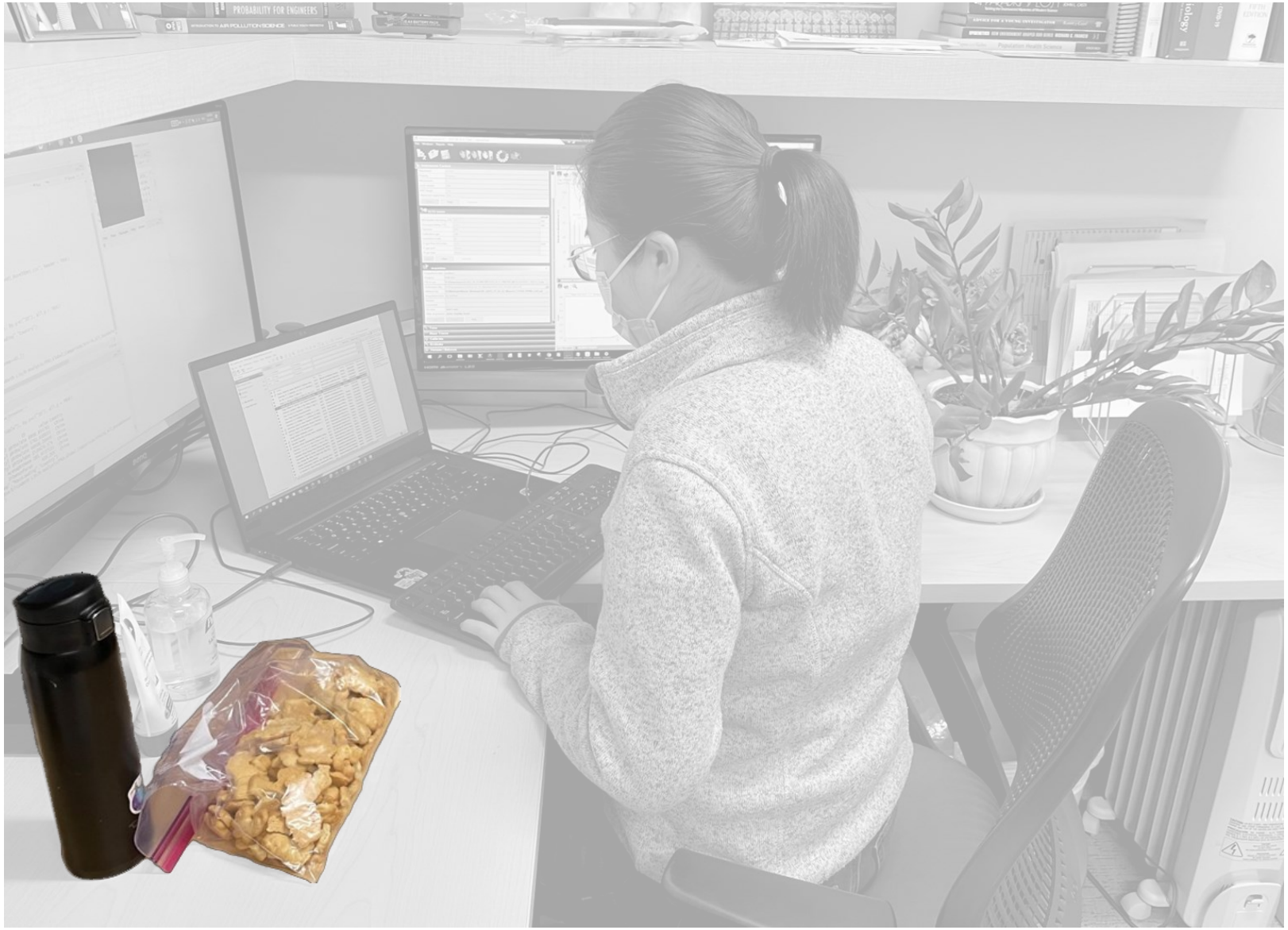
Why Indoor Chemistry Matters Workshop 2
Prioritizing Indoor Chemistry Research

February 8, 2024

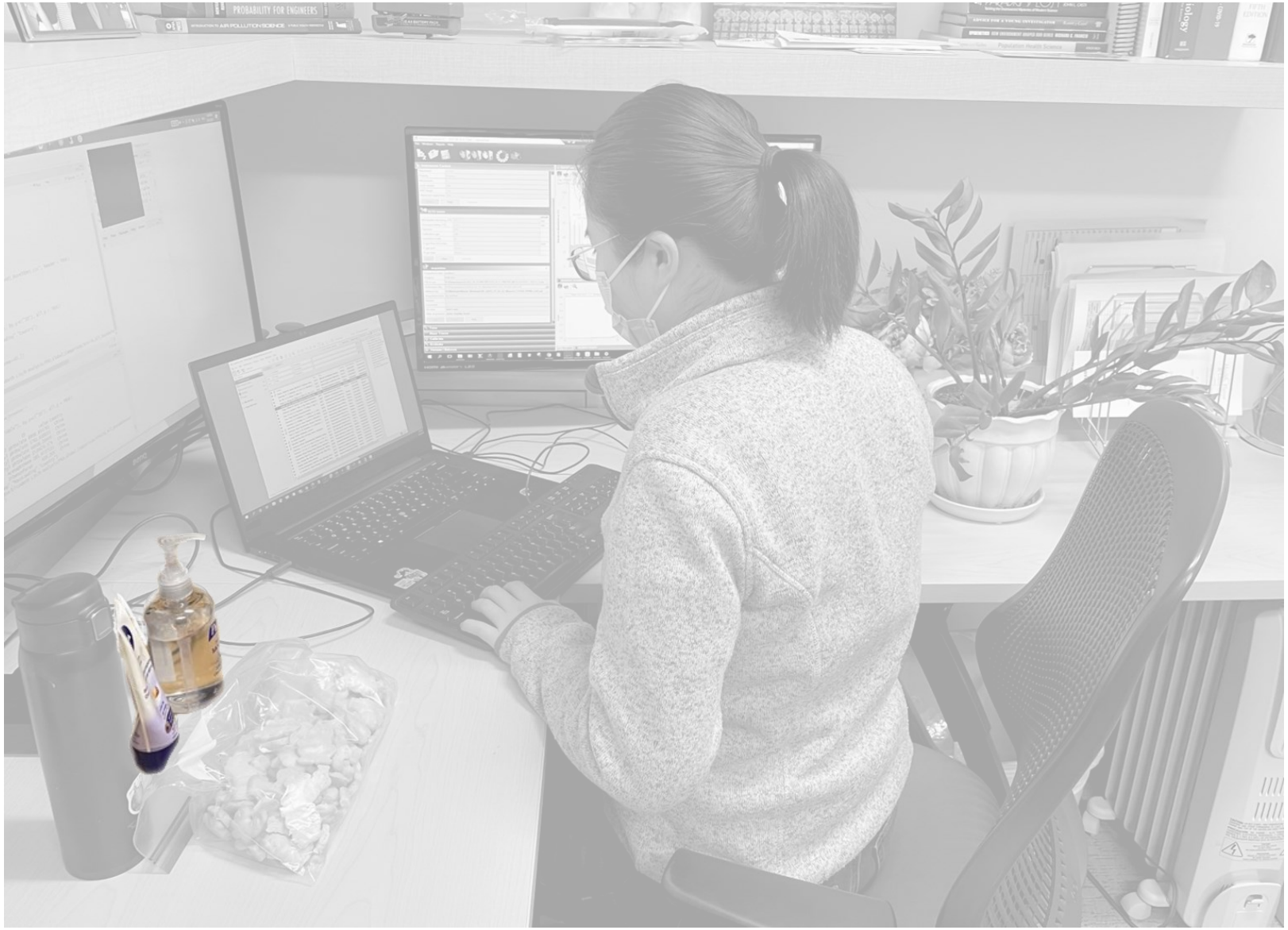
What are you exposed to indoors?



Exposures through ingestion?

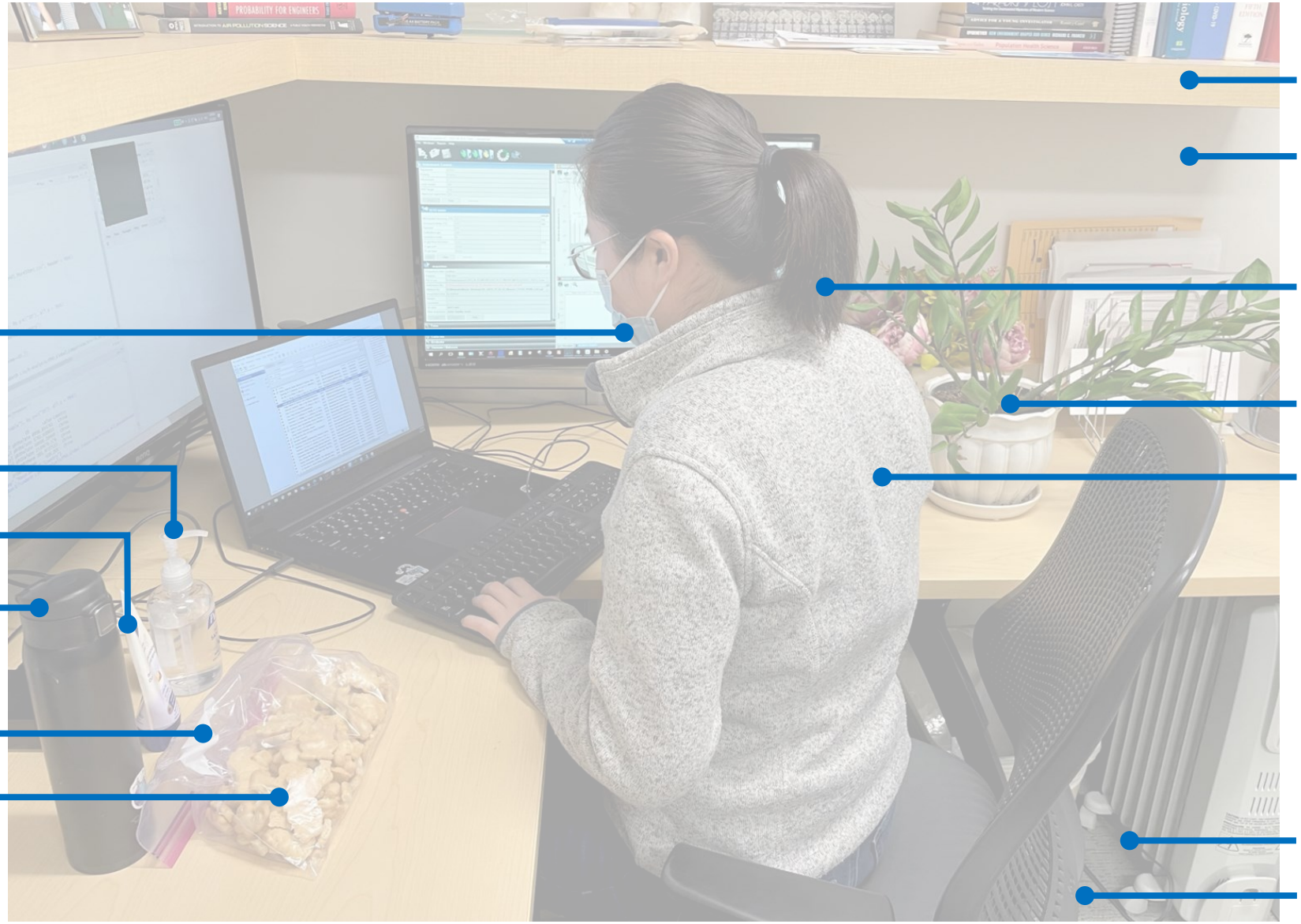


Exposures through dermal contact?



Exposures through inhalation?

MANY sources of particle & gas-phase chemicals



Smoking

Vehicles

Cooking

Pharmaceuticals

Cleaning products

Fragrances

Water contaminants

Plastics

Food products, additives, preservatives

Furnishings

Building materials, paint

Personal care products

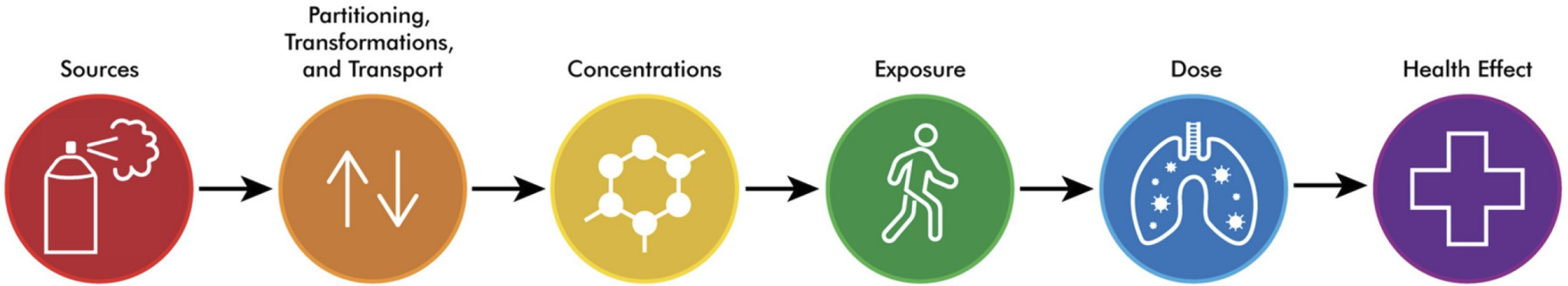
Pesticides

Textiles, colourants

Resuspended Dust

Carpet

How do environmental factors impact health?



National Academies of Sciences, Engineering, and Medicine. 2022. Why Indoor Chemistry Matters. Washington, DC: The National Academies Press.

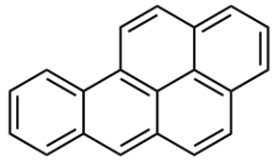
Indoor exposures are:

#1 chemically diverse

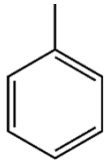
#2 spatially variable with differences within and between individual households

#3 dynamic, influenced by the occupant practices, consumer product use, and behaviour

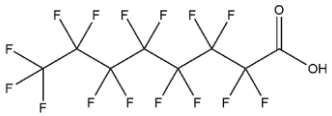
Capturing the human experience using silicone films



POLYCYCLIC AROMATIC HYDROCARBONS (PAHs)

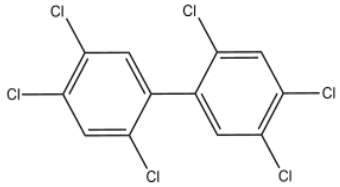


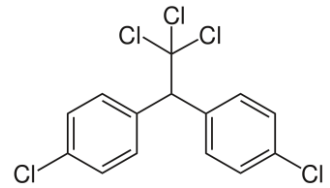
VOLATILE ORGANIC COMPOUNDS (VOCs)



PER-AND POLYFLUOROALKYL SUBSTANCES (PFAS)

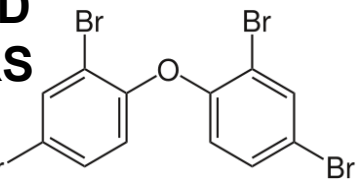
POLYCHLORINATED BIPHENYLS (PCBs)



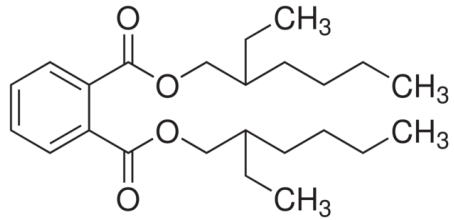


PESTICIDES

POLYBROMINATED DIPHENYL ETHERS (PBDEs)

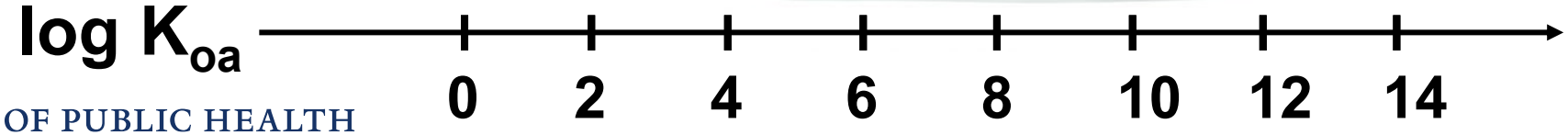


PHTHALATES

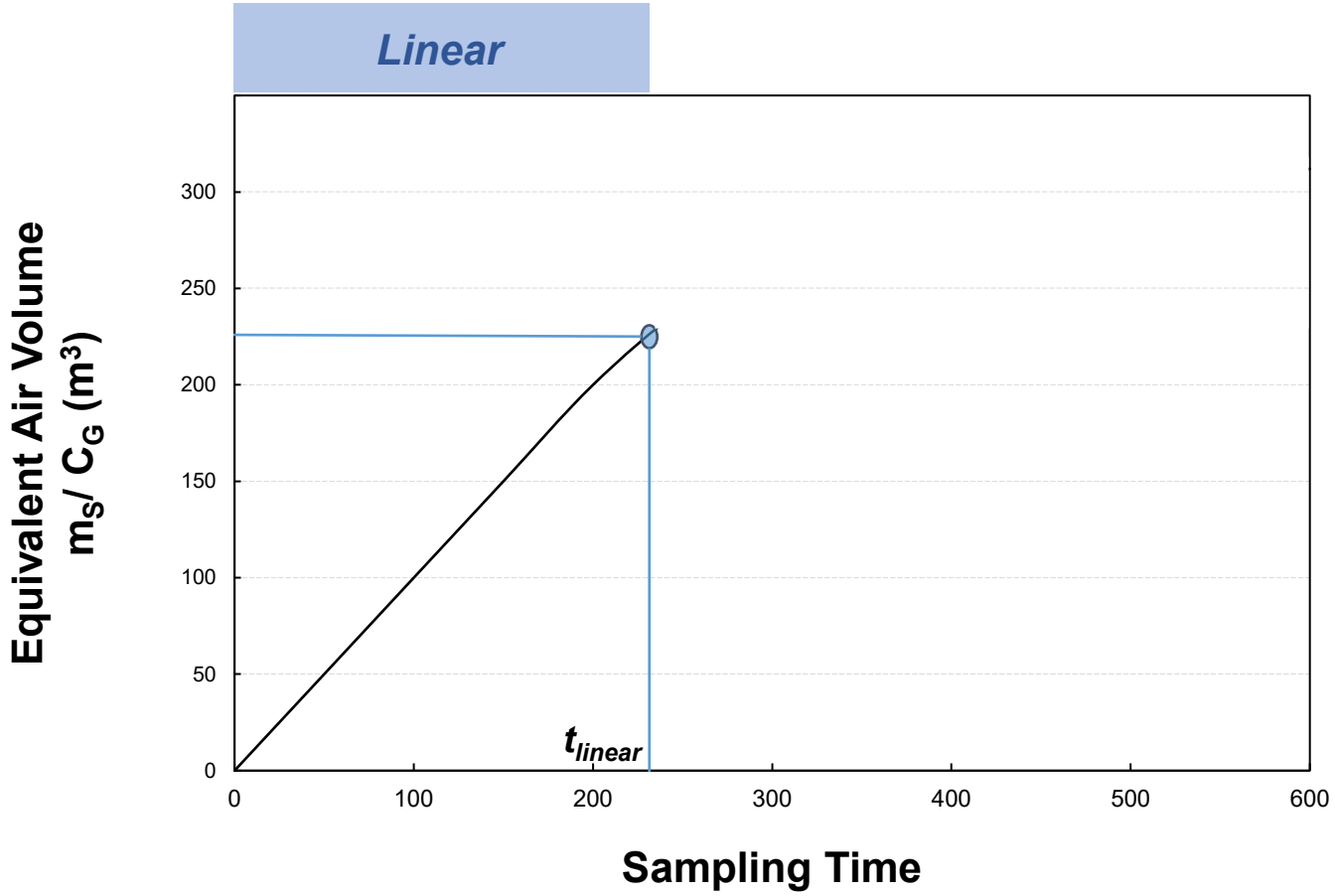


Sorption properties of PDMS are proportional to octanol air partitioning coefficient (log K_{oa})

Polydimethylsiloxane (PDMS)

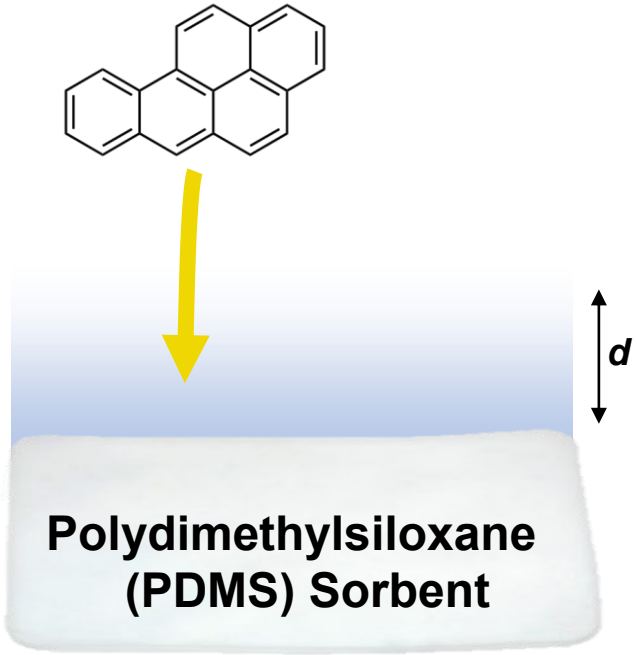


Sampling behaviour of gas-phase chemicals by passive samplers

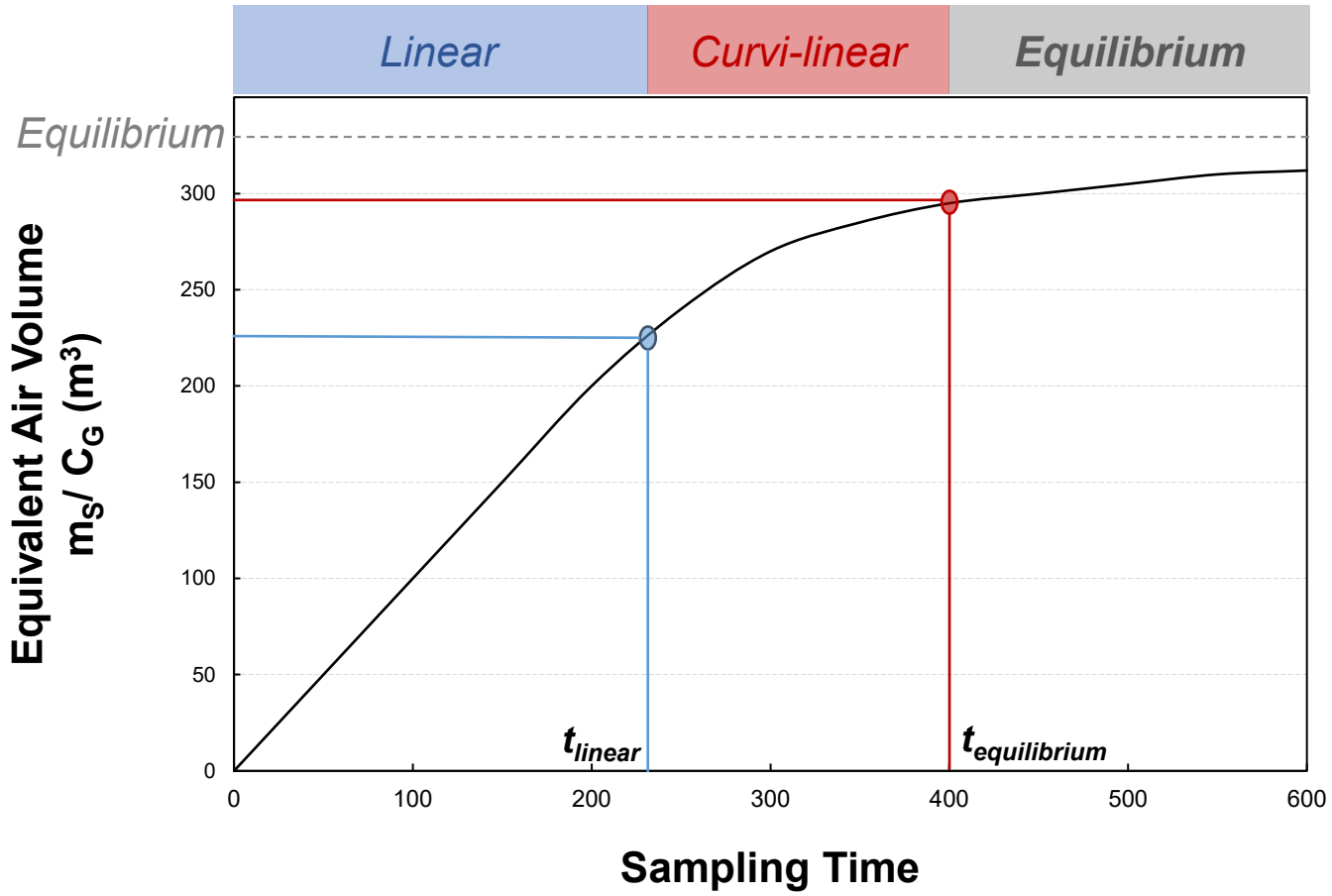


In the **linear phase**, chemical is taken up by a sorbent over time at a constant rate.

The uptake rate depends on the thickness of boundary layer (*d*) above the sorbent.

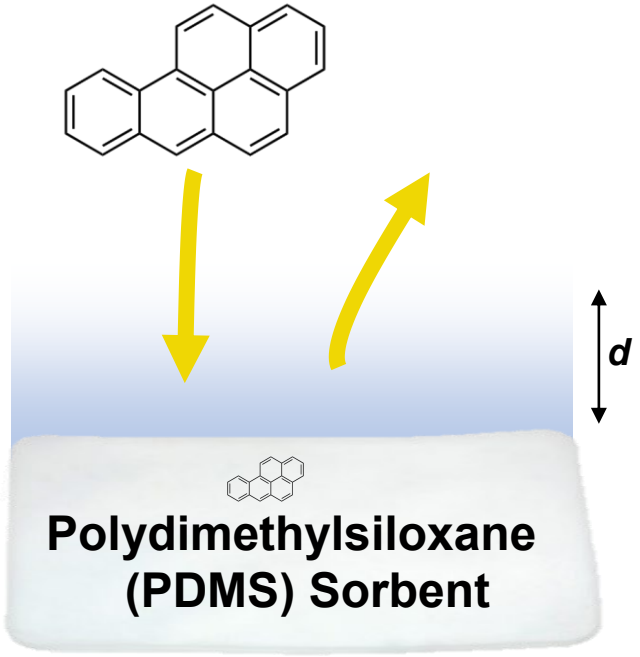


Sampling behaviour of gas-phase chemicals by passive samplers

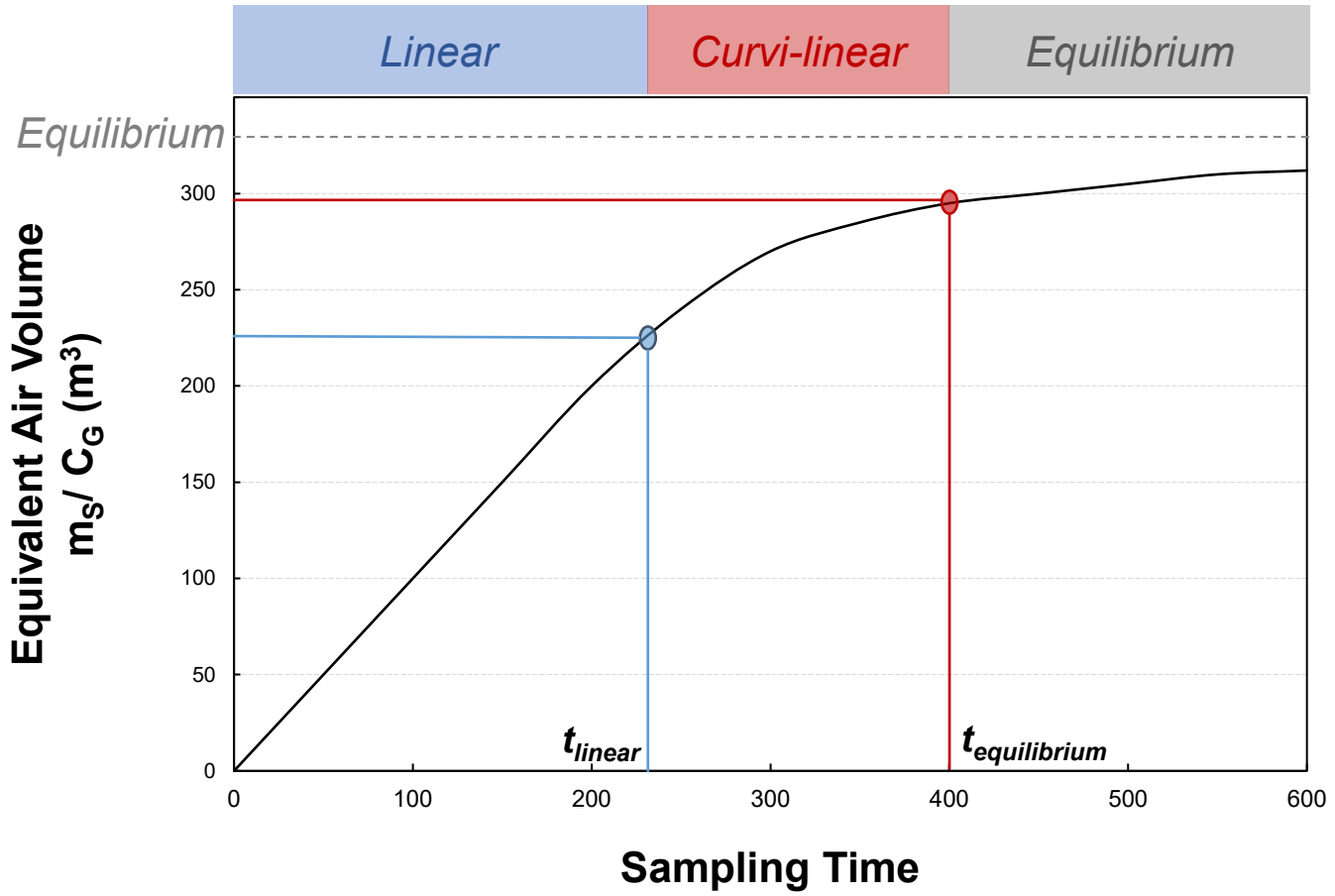


In the **equilibrium phase**, the uptake rate equals the loss rate.

This rate is controlled by the partitioning between the sorbent and air for the chemical.

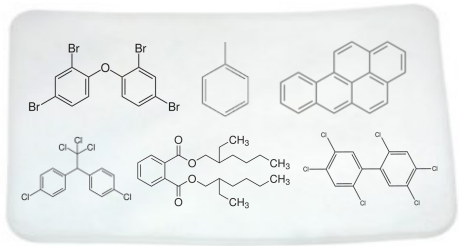


Sampling behaviour of gas-phase chemicals by passive samplers



Measurement of Contaminant Mass Loading
(pg/ sorbent mass)

Passive Sampler Sorbent



Conversion of Mass Loading to Concentration
(m^3/ day)

- **Linear**
  Uptake rate
- **Equilibrium**
  Equilibrium sorption coefficient

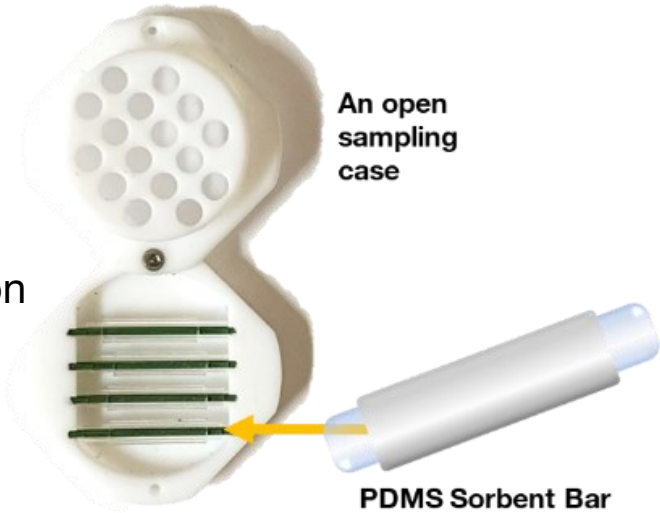
Exposure Concentration
(pg/ m^3)

Wearable Passive Samplers to Assess Personal Exposures

Clip
Fixed Indoor or Outdoor Location

Wristband
Children, Adults

Ankle Band
Infants



Use of the case allows for:

1) *Exclusive sampling of air contaminants*
2) *Constant boundary layer over the sorbent*
3) *Quantification of exposure concentration (pg/m^3)*

High Throughput Chemical Analysis

1. Personal Sampling

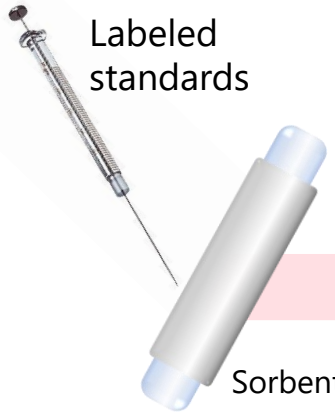
2. Sample preparation (thermal desorption, solvent extraction)

3. Separation by gas chromatography

4. Detection by high resolution Orbitrap mass spectrometry

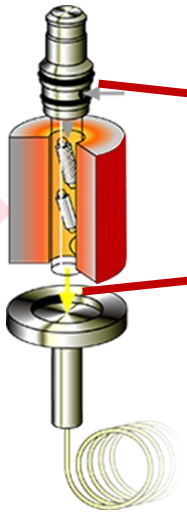
5. Data processed for Exposure Assessment

Wearable passive sampler is typically worn for 1-14 days



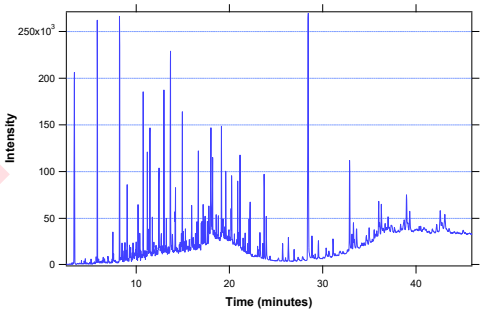
Labeled standards

Sorbent bar



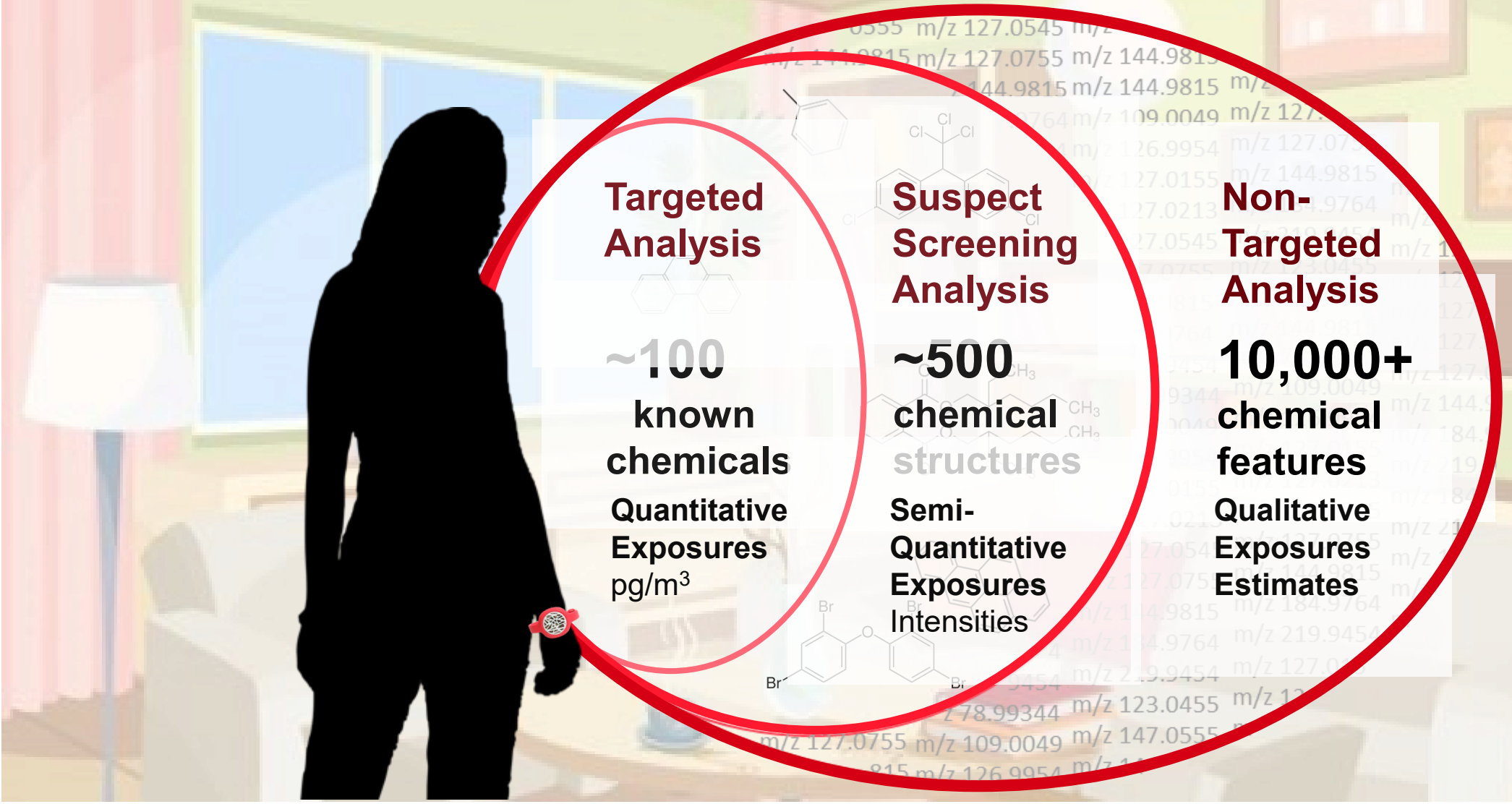
Thermal desorption (300 °C)

Q-Exactive GC Orbitrap MS



Lin *et al.* (2020) *ES&T Letters.* 7(5):308.

Rigorous Computational Workflows for Data Processing



Koelmel *et al.* (2021) *ES&T.* 55(6):3796.

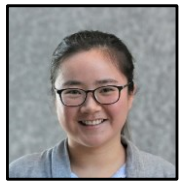
Indoor exposures are:

#1 chemically diverse

#2 spatially variable with differences within and between individual households

#3 dynamic, influenced by the occupant practices, consumer product use, and behaviour

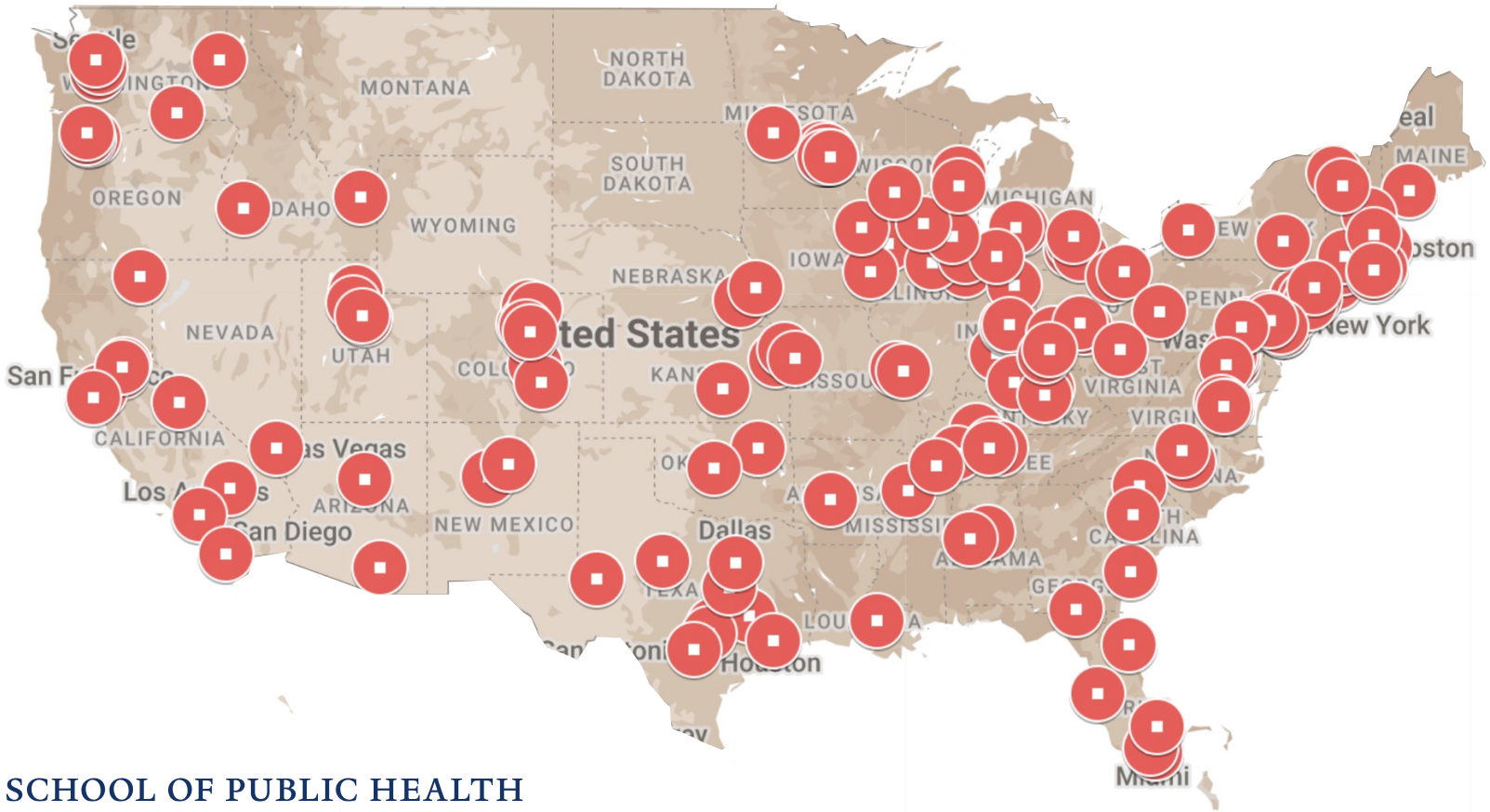
Measuring indoor air across the US



PRESTO
BOSTON UNIVERSITY

Pregnancy Study Online (PRESTO), an internet-based preconception cohort study

- Wristband worn by 139 female participants that were all trying to conceive
- Aged 21 to 45 years
- June to November 2021



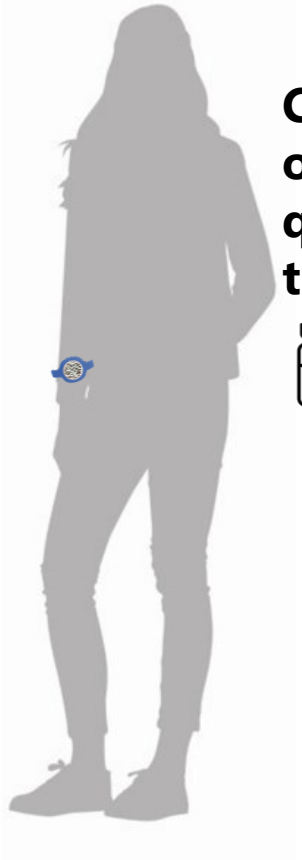
Participants were from 39 states

Wristband worn for 5 days

Self-reported questionnaire detailing household characteristics and activity patterns

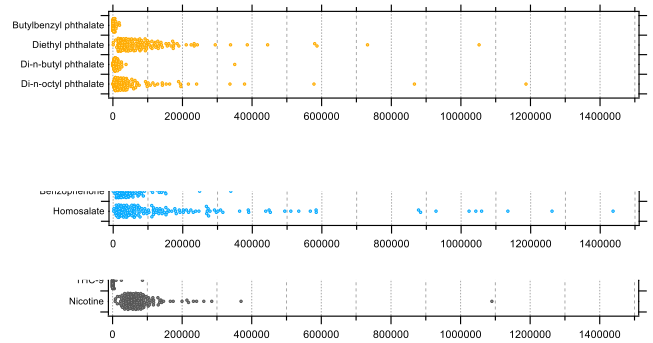
Participants stayed indoors for >90% of the time the wristband was worn.

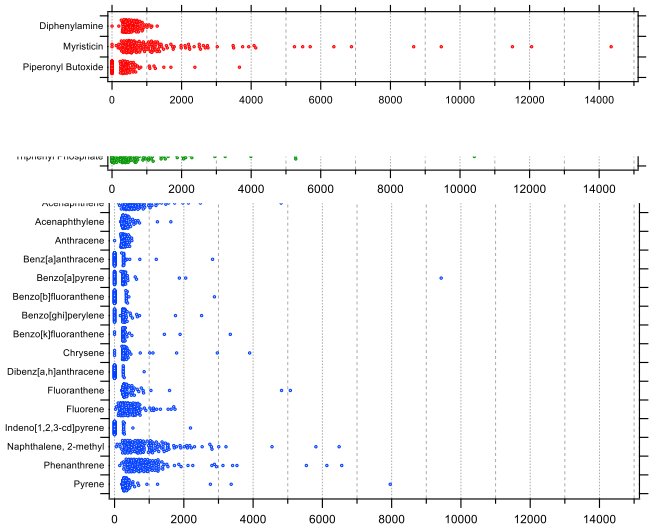
Chemicals recognized to impact health are detected in homes across the US



Concentrations of 81 chemicals quantified across the cohort

Targeted





		Detection Frequency
Phthalates	Butylbenzyl phthalate	77%
	Diethyl phthalate	100%
	Di-n-butyl phthalate	100%
	Di-n-octyl phthalate	100%
Cosmetics	Benzophenone	100%
	Homosalate	100%
	TNCS	100%
Smoking-related	Nicotine	15%
	TNCS	100%
Pesticides	Diphenylamine	99%
	Myristicin	100%
	Piperonyl Butoxide	56%
Flame Retardants	Triphenyl Phosphate	74%
Combustion -related	Acenaphthylene	100%
	Anthracene	100%
	Benz[a]anthracene	100%
	Benzo[a]pyrene	100%
	Benzo[b]fluoranthene	100%
	Benzo[ghi]perylene	19%
	Benzo[k]fluoranthene	60%
	Chrysene	9%
	Dibenz[a,h]anthracene	100%
	Fluoranthene	100%
	Fluorene	6%
	Indeno[1,2,3-cd]pyrene	100%
	Naphthalene, 2-methyl	100%
	Phenanthrene	8%
	Pyrene	100%

0 200 400 600 800 1000 1200 1400

2 4 6 8 10 12 14

Concentration (ng/m³)

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Chemicals in indoor air originate from a myriad of sources and are biologically relevant

491 unique chemicals identified

Suspect Screening

SCIENTIFIC DATA

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

The EPA CompTox Dashboard was used to screen chemicals usage and hazards

Dionisio et al (2018) Scientific Data. 5:18038.
https://comptox.epa.gov/dashboard/

Possible Products/Uses

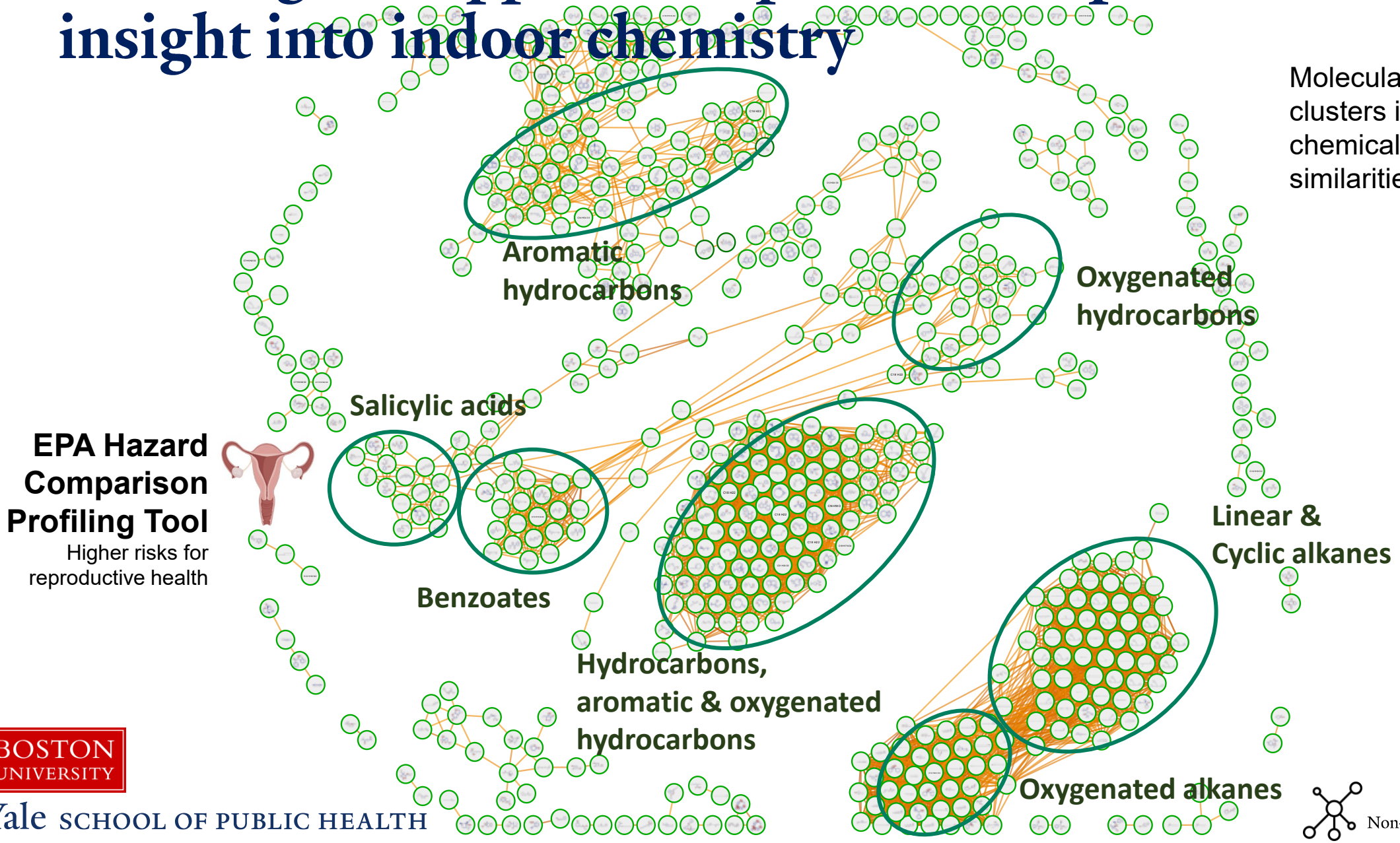
118 cosmetics
79 food-related
62 flavourants
35 pharmaceuticals
17 combustion products
15 pesticides
4 antimicrobials
3 smoking-related

Predicted Toxicity

Carcinogenic	24 chemicals
Genotoxic or Mutagenic	324 chemicals
Endocrine Disruption	361 chemicals
Developmental	359 chemicals
Reproductive	68 chemicals

Non-targeted approaches provide comprehensive insight into indoor chemistry

Molecular network clusters indicate chemicals with structural similarities.

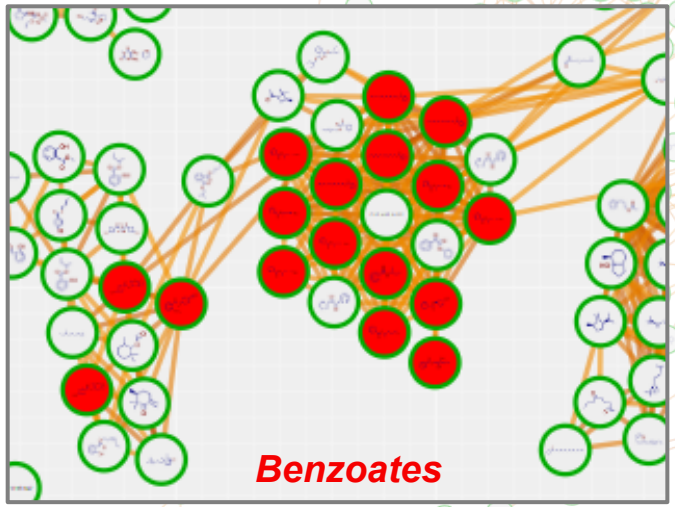


EPA Hazard Comparison Profiling Tool

Higher risks for reproductive health

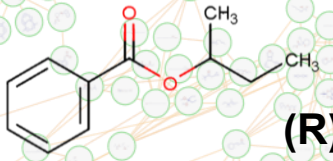
Identification of emerging chemicals in the air

The compounds shown in red have potential sources.

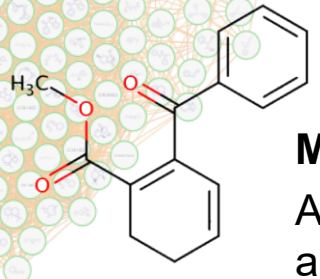


Benzoate cluster

Dodecyl benzoate
Emollient in cosmetic products

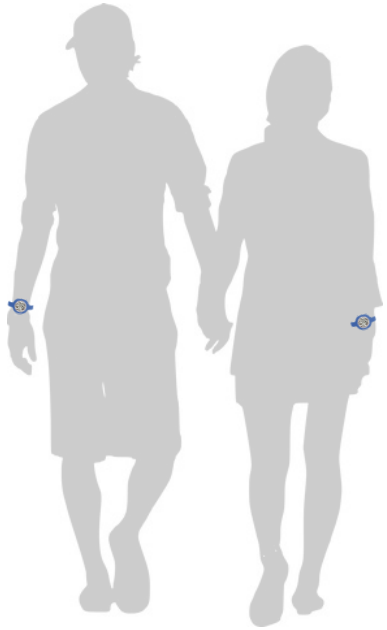


(R)-sec-butyl benzoate
Preservative in commercial cosmetic lotions



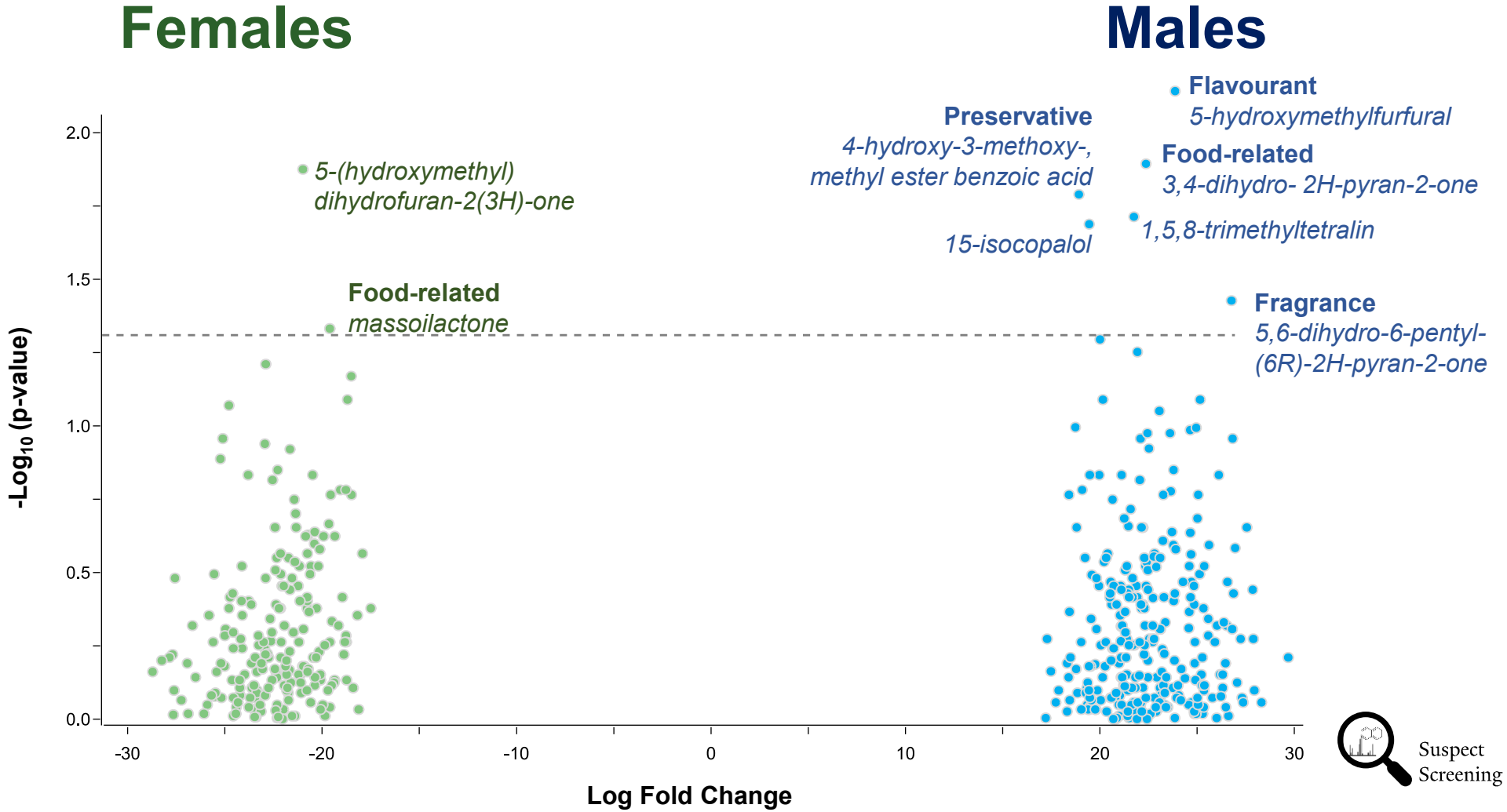
Methyl o-benzoylbenzoate
Anti-ultraviolet absorber and
a preservative in foods and beverages

Difference in consumer product use can lead to distinct personal exposures within a household



24 female-male partners worn the wristband over the same 7-day period

Couples were from 17 states



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Suspect Screening

Indoor exposures are:

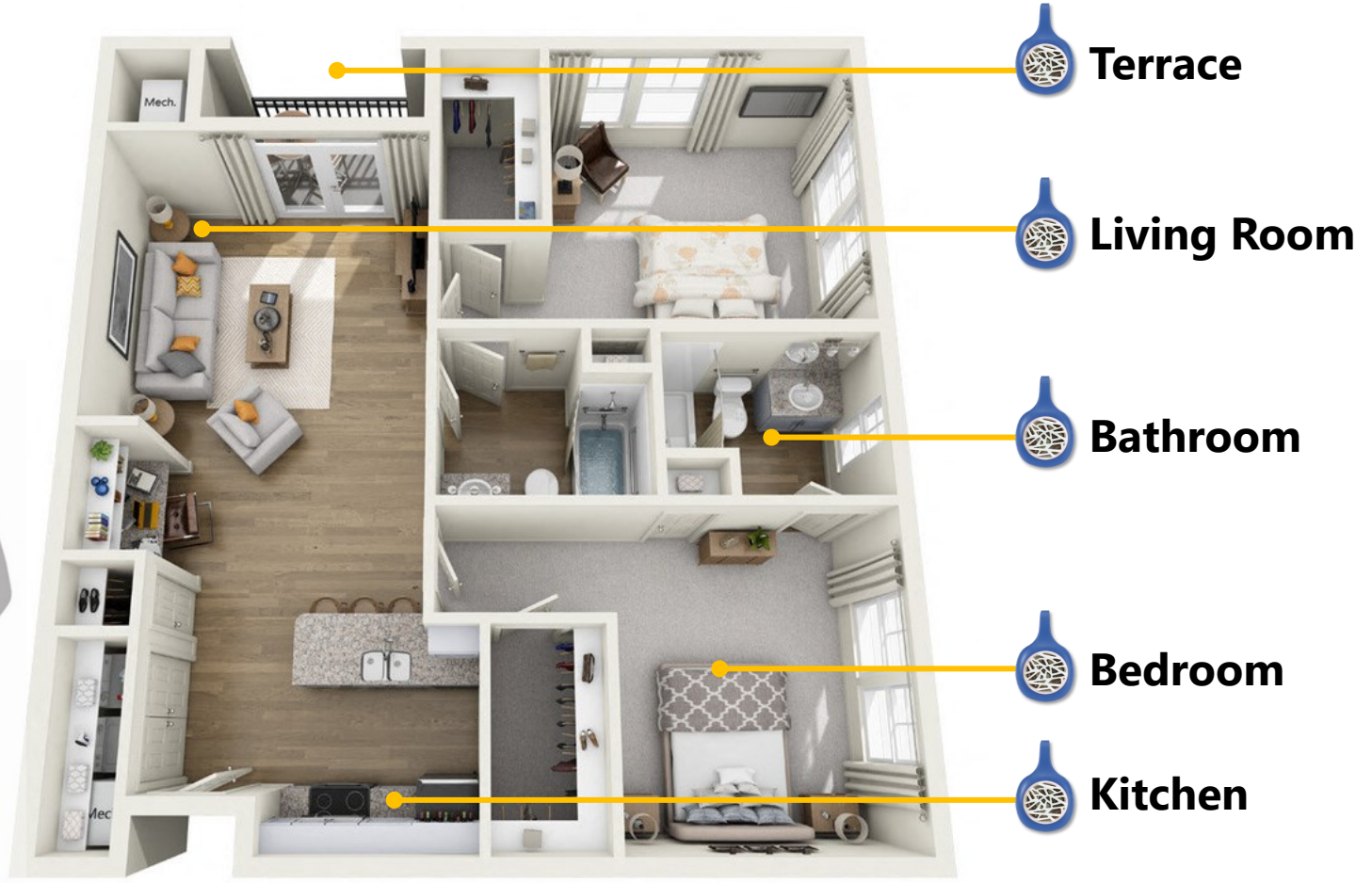
#1 chemically diverse

#2 spatially variable with differences within and between individual households

#3 dynamic, influenced by the occupant practices, consumer product use, and behaviour

Measuring indoor air across a household

- Air monitoring in 37 homes in Switzerland
- Participants were all non-smoking adults (21- 58 years)
- 6 samples collected from each home (1 personal, 5 stationary) over 3 days
- October to December 2021



EPFL

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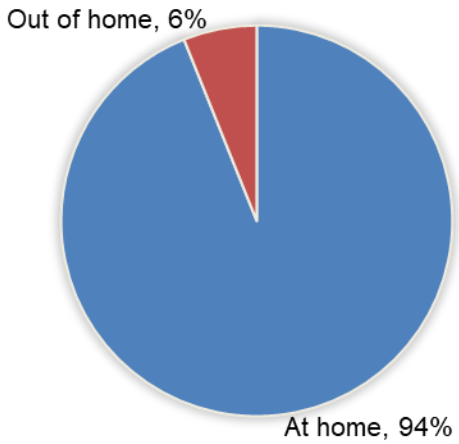
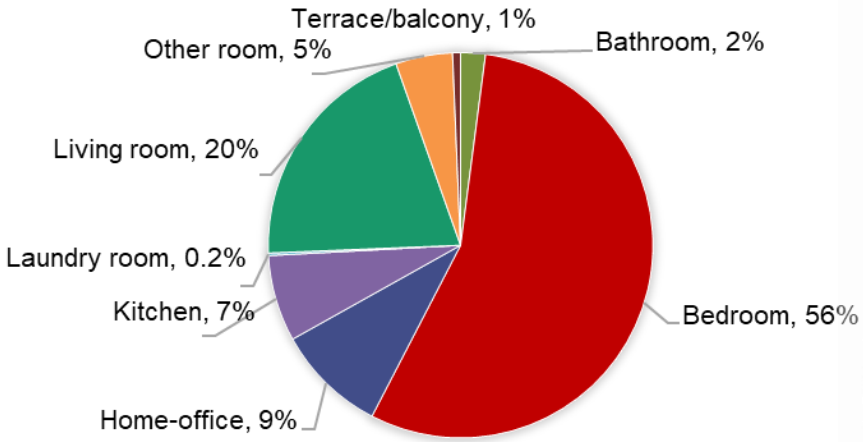
González Serrano *et al.* (2021) *Environ. Res.* 231(Pt 2):116197.

Measuring indoor air across a household

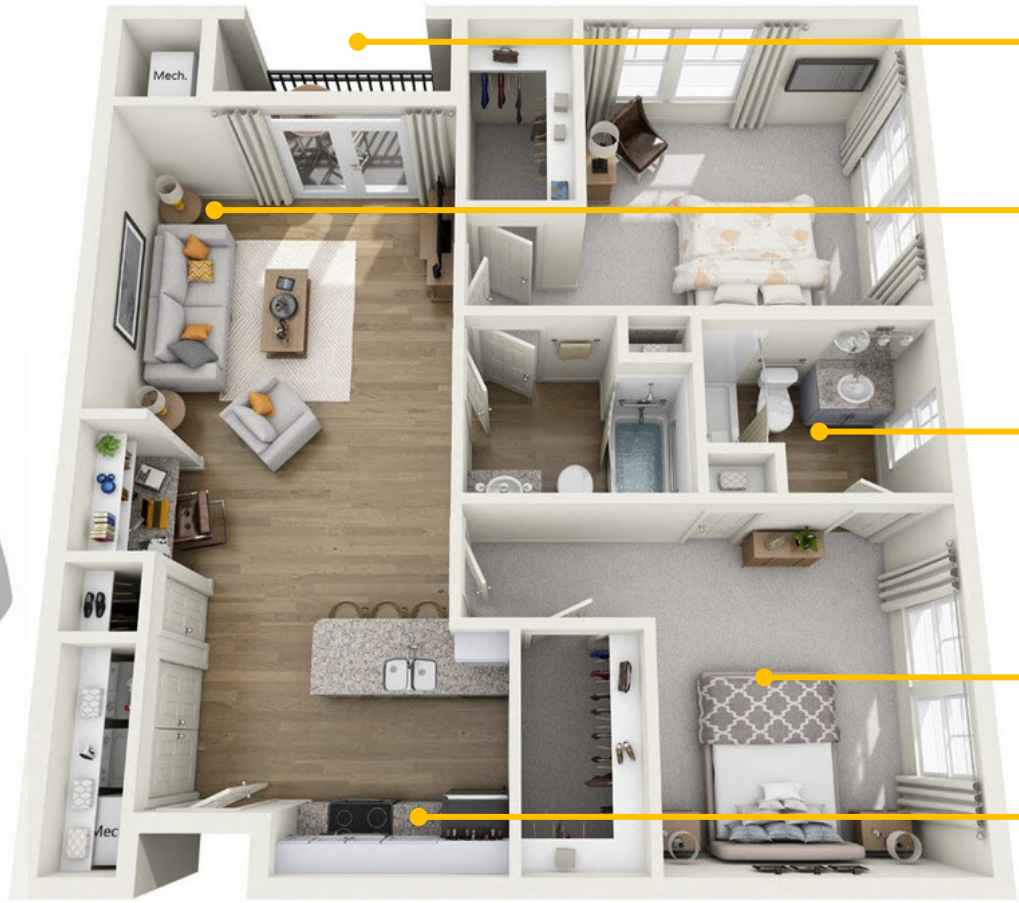
TIME SPENT INSIDE THE HOME



TIME-ACTIVITY BUDGET



Personal



Terrace

Living Room

Bathroom

Bedroom

Kitchen

EPFL

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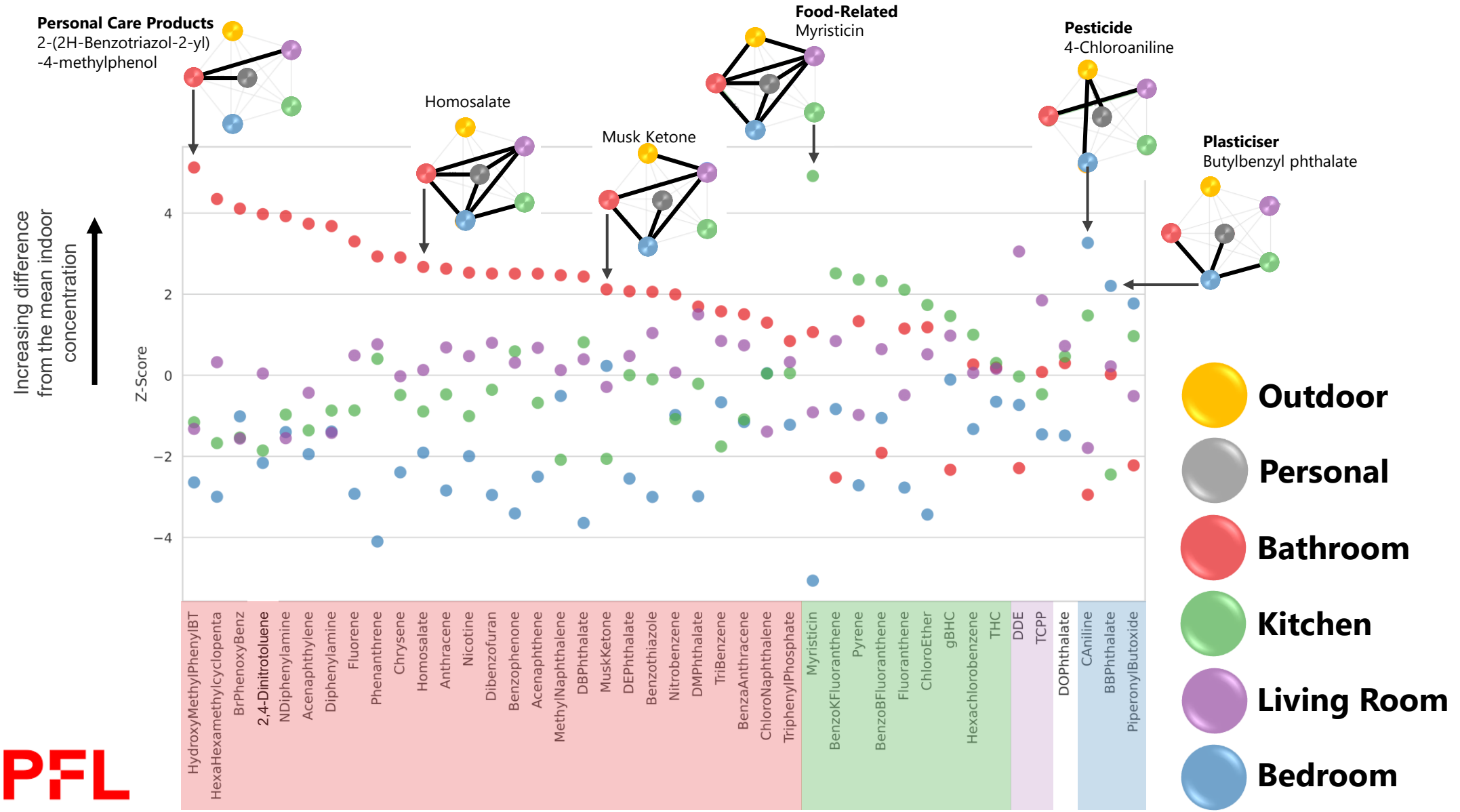
González Serrano *et al.* (2021) *Environ. Res.* 231(Pt 2):116197.

How do we interact with our indoor spaces?



EPFL

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Targeted

Indoor exposures are:

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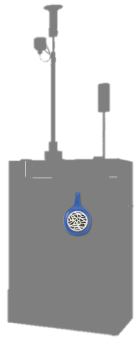
Measuring indoor air longitudinally

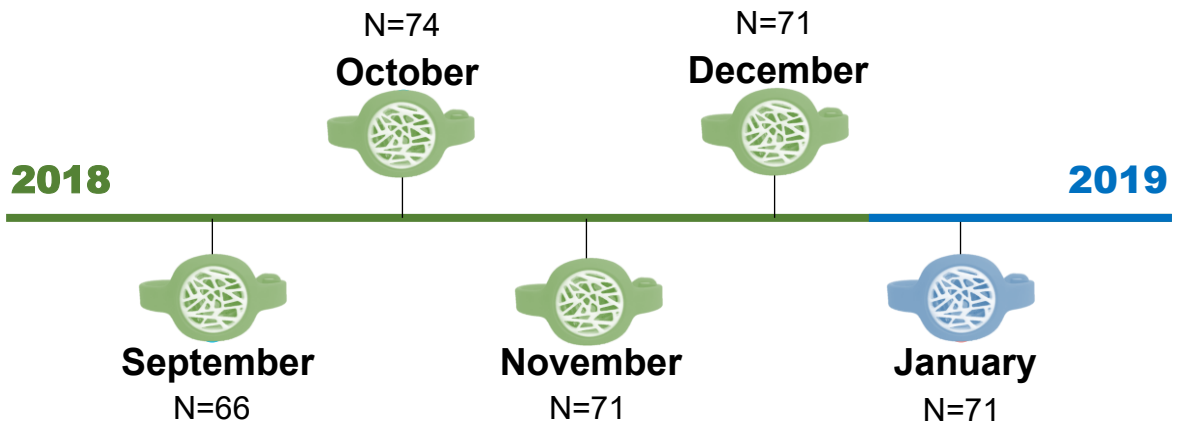
3 days

Personal Monitoring



3 days

Outdoor Monitoring



Parallel outdoor air sampling was conducted over the study period.

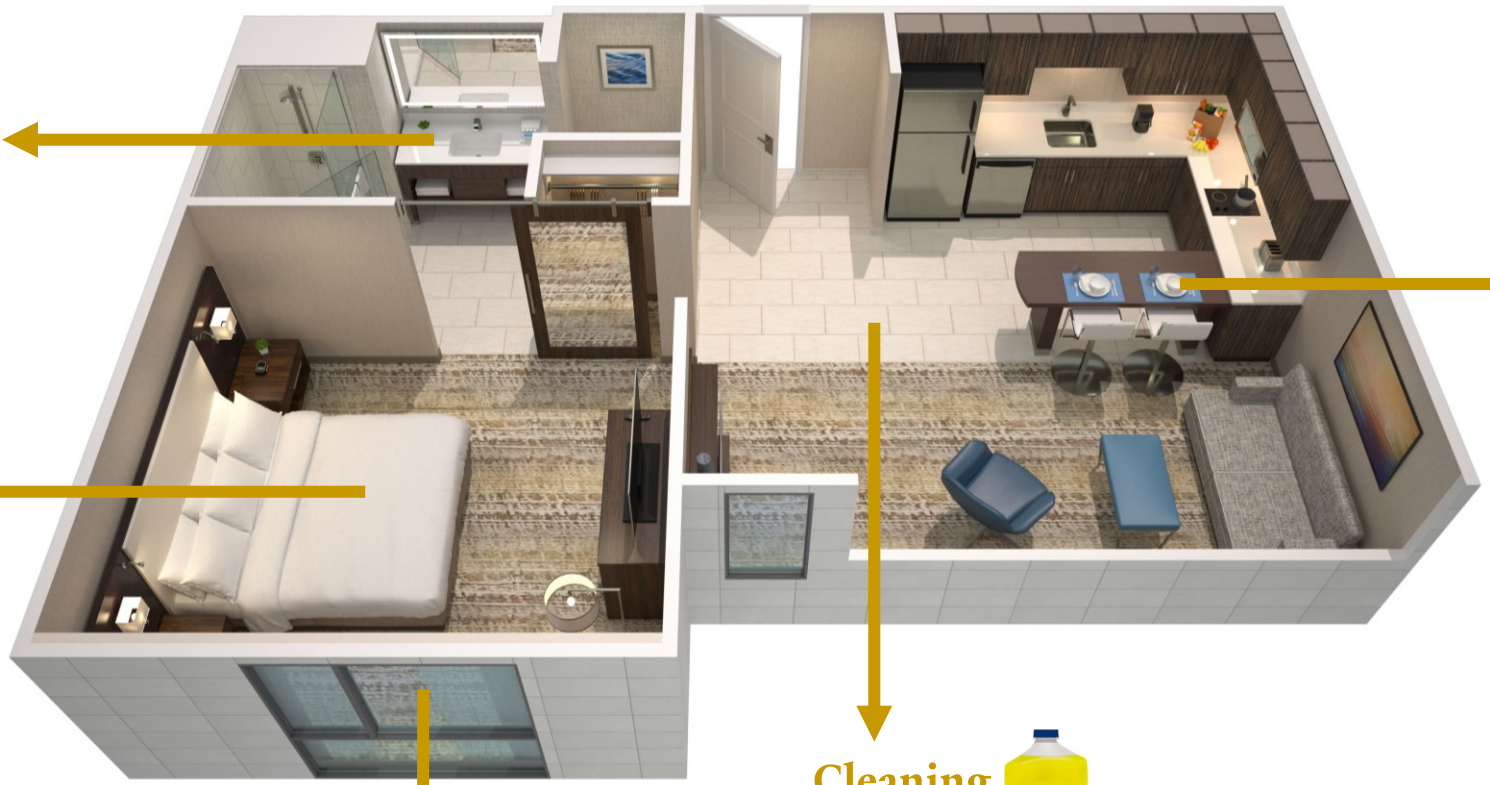
Jinan, China
Adults (60-69 years)

Biomarkers of **A**ir **P**ollutants **E**xposure (**China BAPE**) Study

Guo *et al.* (2021) *Environment International*. 156:106709.
Koelmel *et al.* (2021) *Environmental Pollution.* 270:116228.
Shi *et al.* (2022) *Environment International*. 170:107614.

Tracking time-activity patterns in our homes

Personal Care



Diet

Pest Control

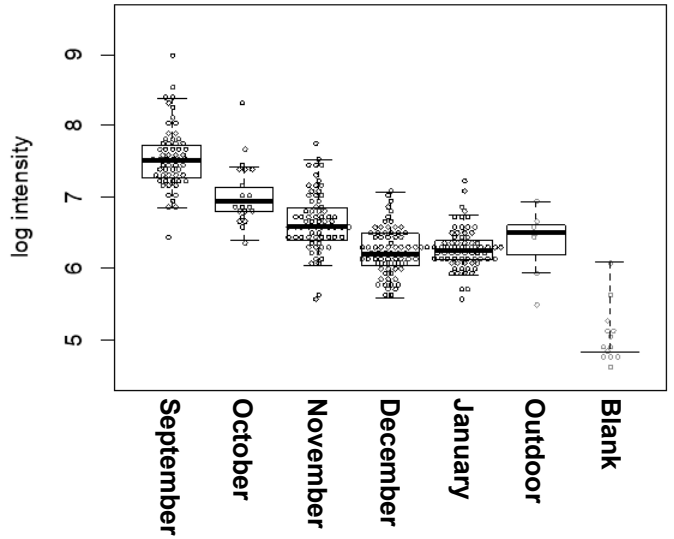
Cleaning Activities

Ventilation Practices

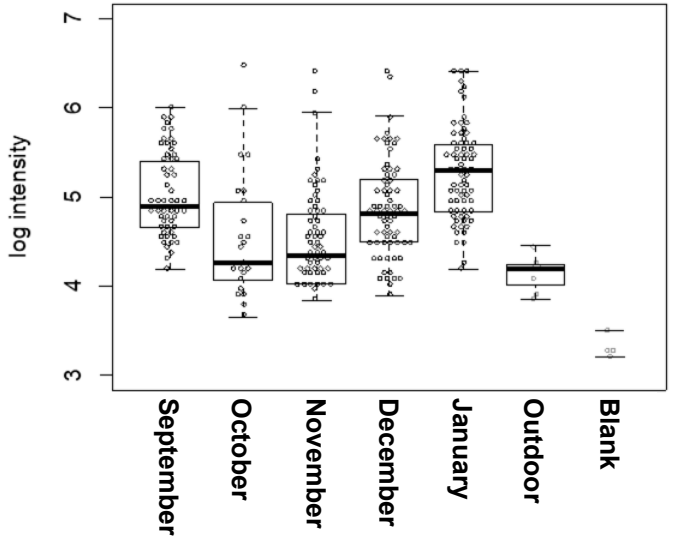
Seasonal Use

*Product for **mosquito control** placed under bed by participants during warmer months*

Dichlorvos



Triclosan



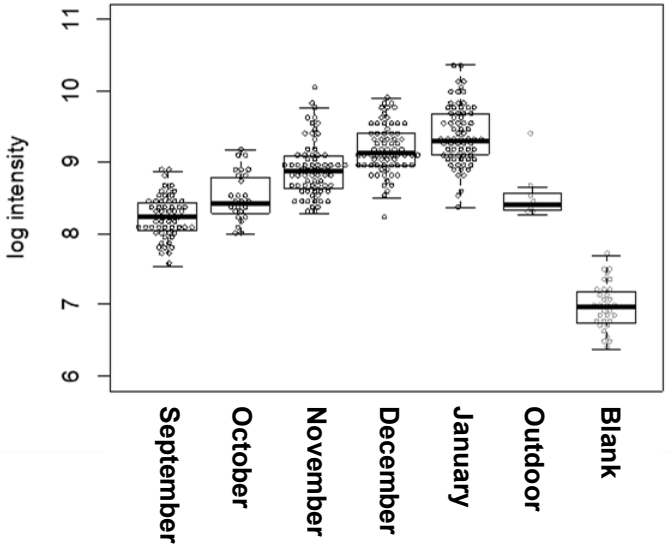
No temporal variance

*Similar **personal care products** used by participants across seasons*

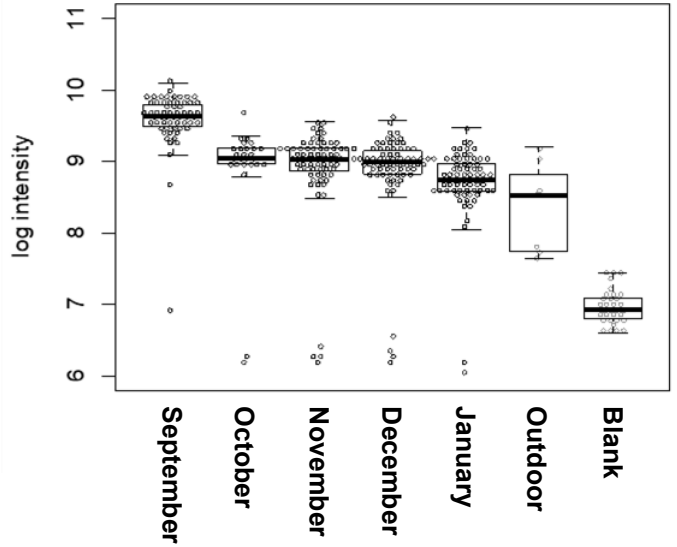
Indoor sources

Chemicals from food and cleaning products increased indoors with decreases ventilation during cooler months

Limonene



BHT (butylated hydroxytoluene)



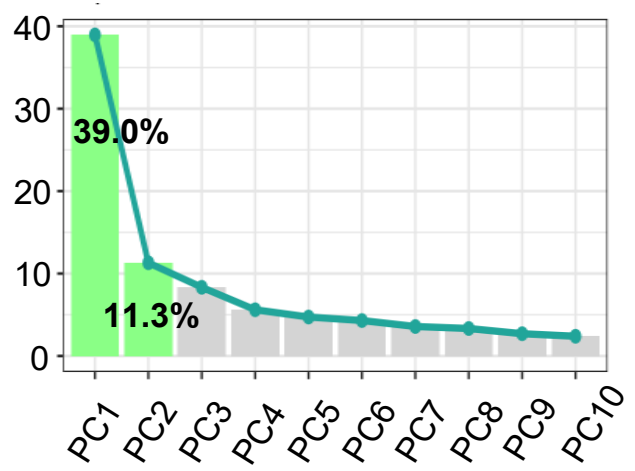
***Food preservative** in grain products found in the controlled diet given to all participants*

Suspect Screening

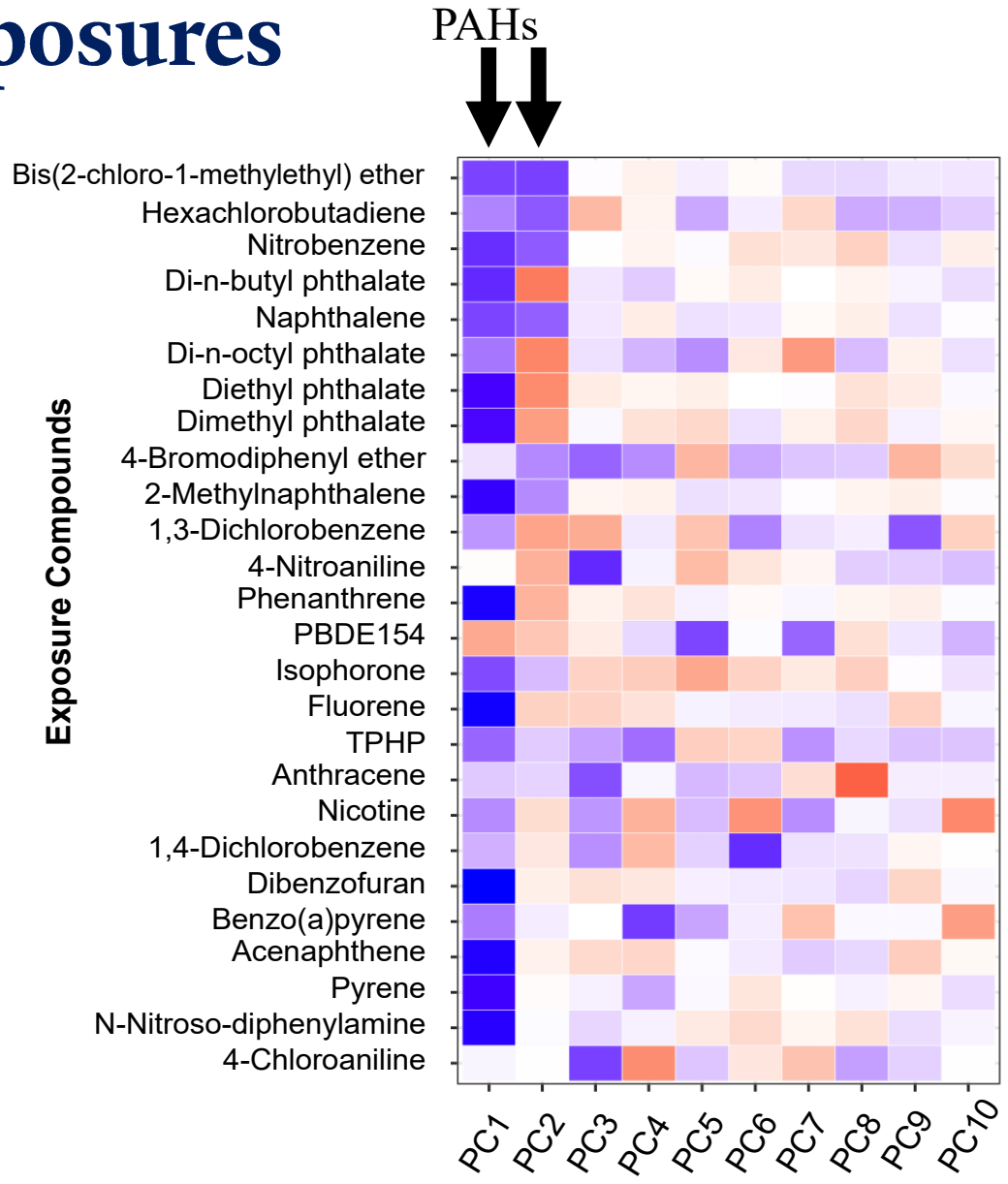
Koelmel *et al.* (2021) *Environmental Pollution.* 270:116228.

Identifying predictors of exposures

Percent Variance Explained



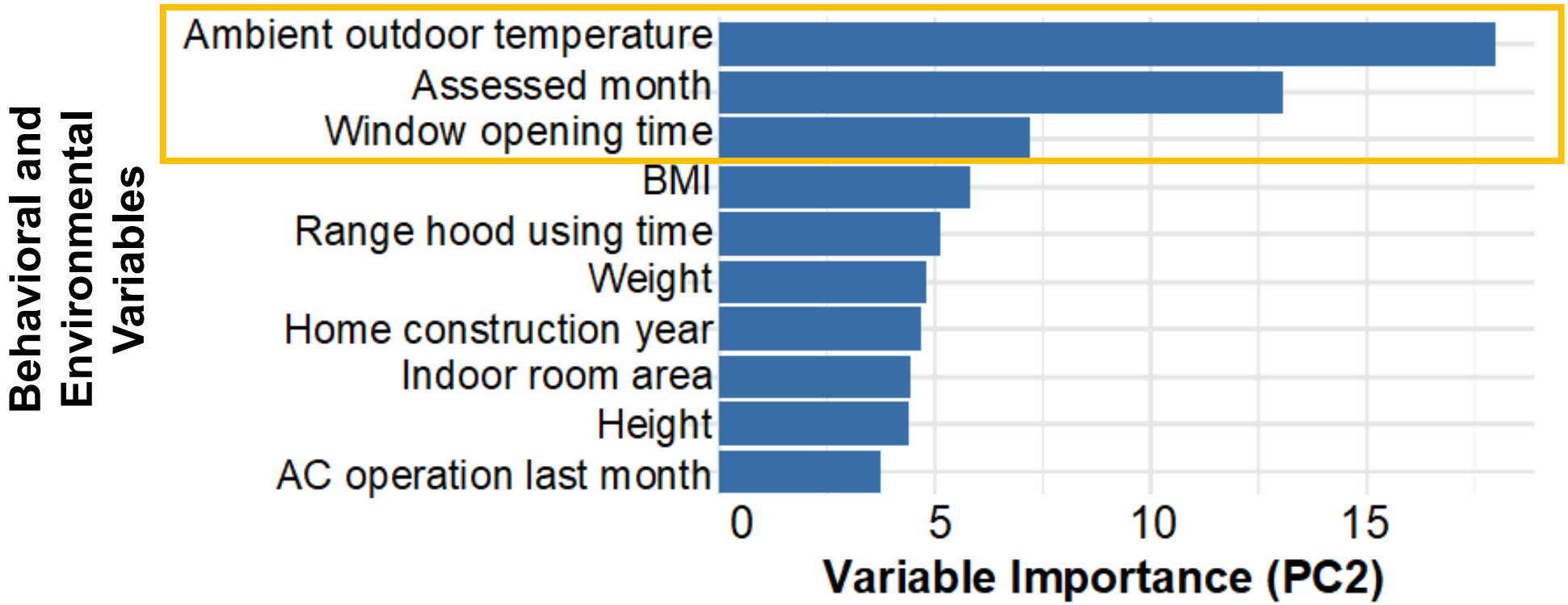
Approximately 50% of variance across exposure compounds explained by two clusters



Targeted

Guo *et al.* (2021) *Environment International*. 156:106709.

Indoor air composition is influenced by our behaviours and environmental factors



Guo *et al.* (2021) *Environment International*. 156:106709.

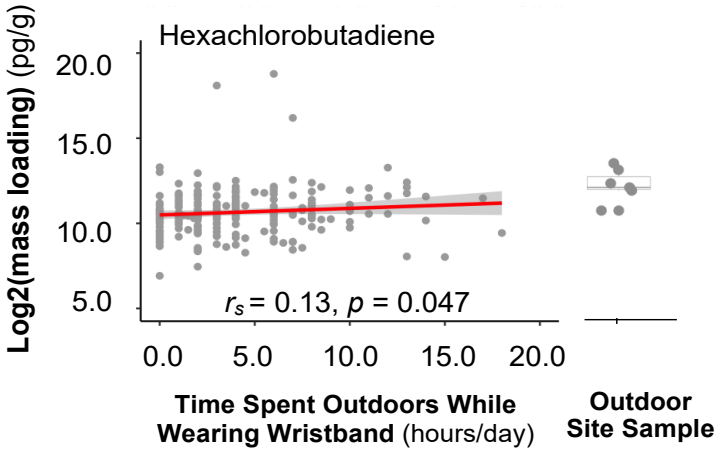
Contribution of indoor vs. outdoor sources to exposures

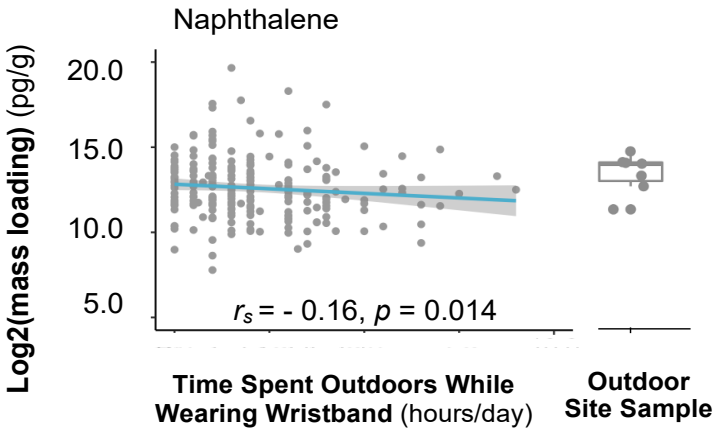
Outdoor Sources

Hexachlorobutadiene
Bis(2-chloro-1-methylethyl) ether

Indoor Sources

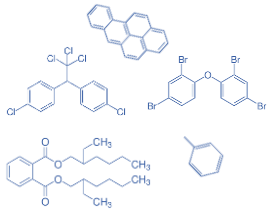
Dieldrin
2,4-Dinitrotoluene
Delta-9-tetrahydrocannabinol
TCPP
Methoxychlor
Naphthalene
Phthalates





Summary

Advances in Measurement Technologies. Wearable and stationary passive samplers coupled with high resolution mass spectrometry provide omic-scale measures of the chemicals in the air. The non-invasive design of these tools has allowed for comprehensive assessment of different indoor environments. Use of a harmonised measurement approach has enabled comparative assessment across geographic settings and populations.



Indoor Air is Chemically Diverse. Non-targeted approaches have revealed hundreds of chemicals in indoor air that are biologically relevant. Findings highlight previously underappreciated sources, exposures, and pathways.

Indoor Air is Dynamic. The behaviour and consumer product use of occupants drive temporal and spatial variability in indoor spaces. The personal exposure of occupants within the same household can differ.

Moving Forward

Data Inconsistencies. A robust, reliable, and rigorous framework for standardised measurement protocols, data collection, and analysis methods (analytical, computational) should be established to define best practices.

Influence on Health. Understanding the impact of complex chemical mixtures (emissions, transformation products) in indoor environments on human health and disease should be prioritised to guide policy decisions.

Exposure Ensemble. Team science using transdisciplinary approaches are necessary to integrate chemical factors with the compilation of *all* physical, biological, and psychosocial influences that impact biology.

Actionable Solutions. There is a need to capture product use and activity patterns across diverse populations (vulnerable, disadvantaged) to understand the influences on indoor chemistry but also enable precision interventions.

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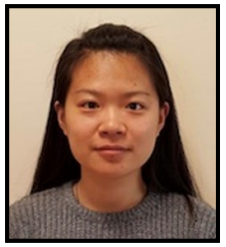

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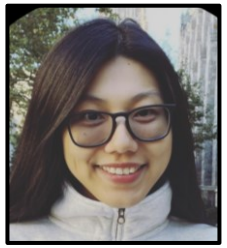

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