Future chemicals of concern: Semi-volatile compounds in the indoor environment

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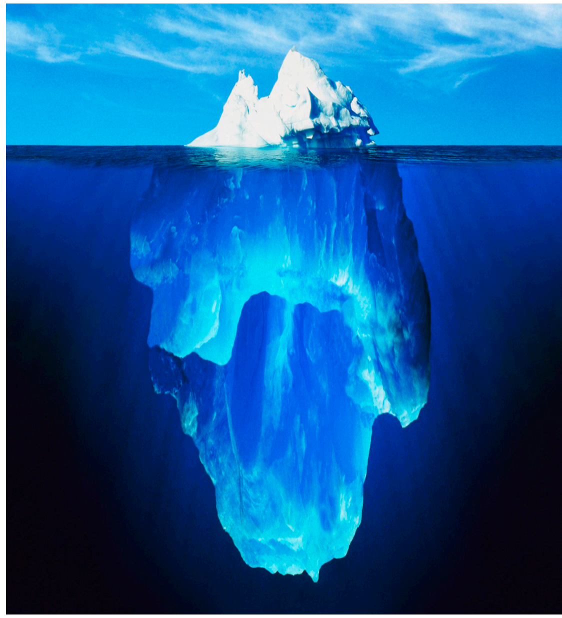
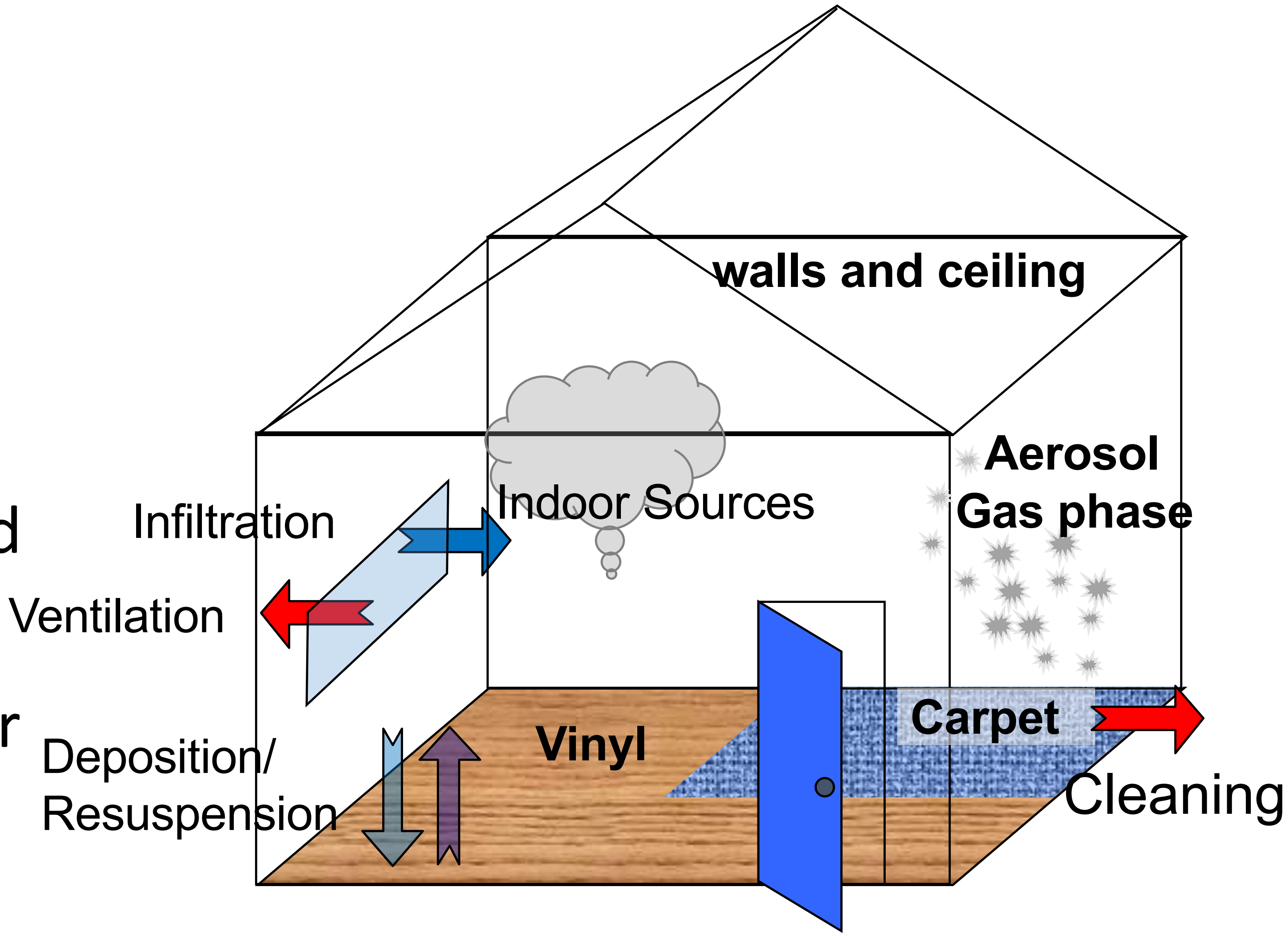
Why semi–volatile compounds?

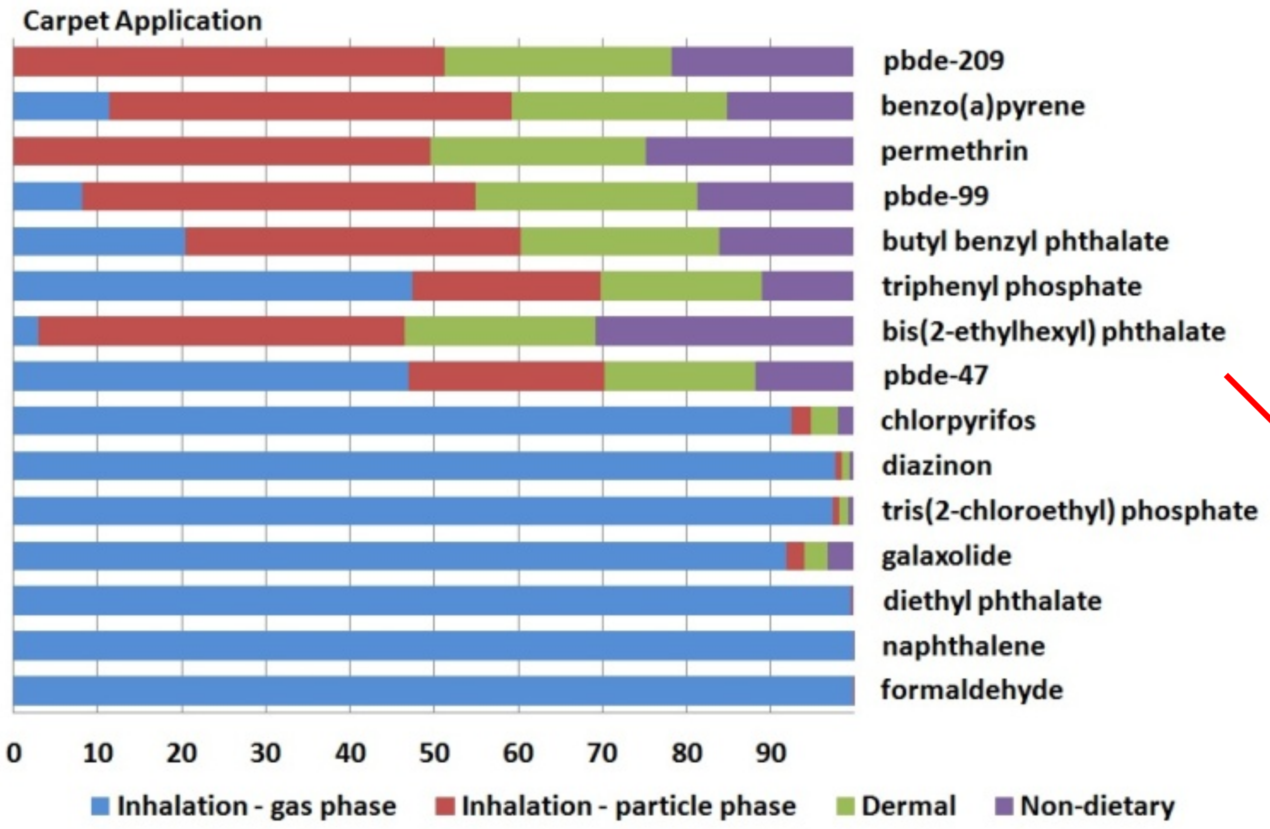
- Exposure to compounds emitted indoors is important
  - Where we spend our time, more exposure per unit emission
- We are not looking at all the relevant compounds
  - Thousands of compounds out there with very little data
- But why should we think about what is in dust?



Dust: Marker of SVOC exposure

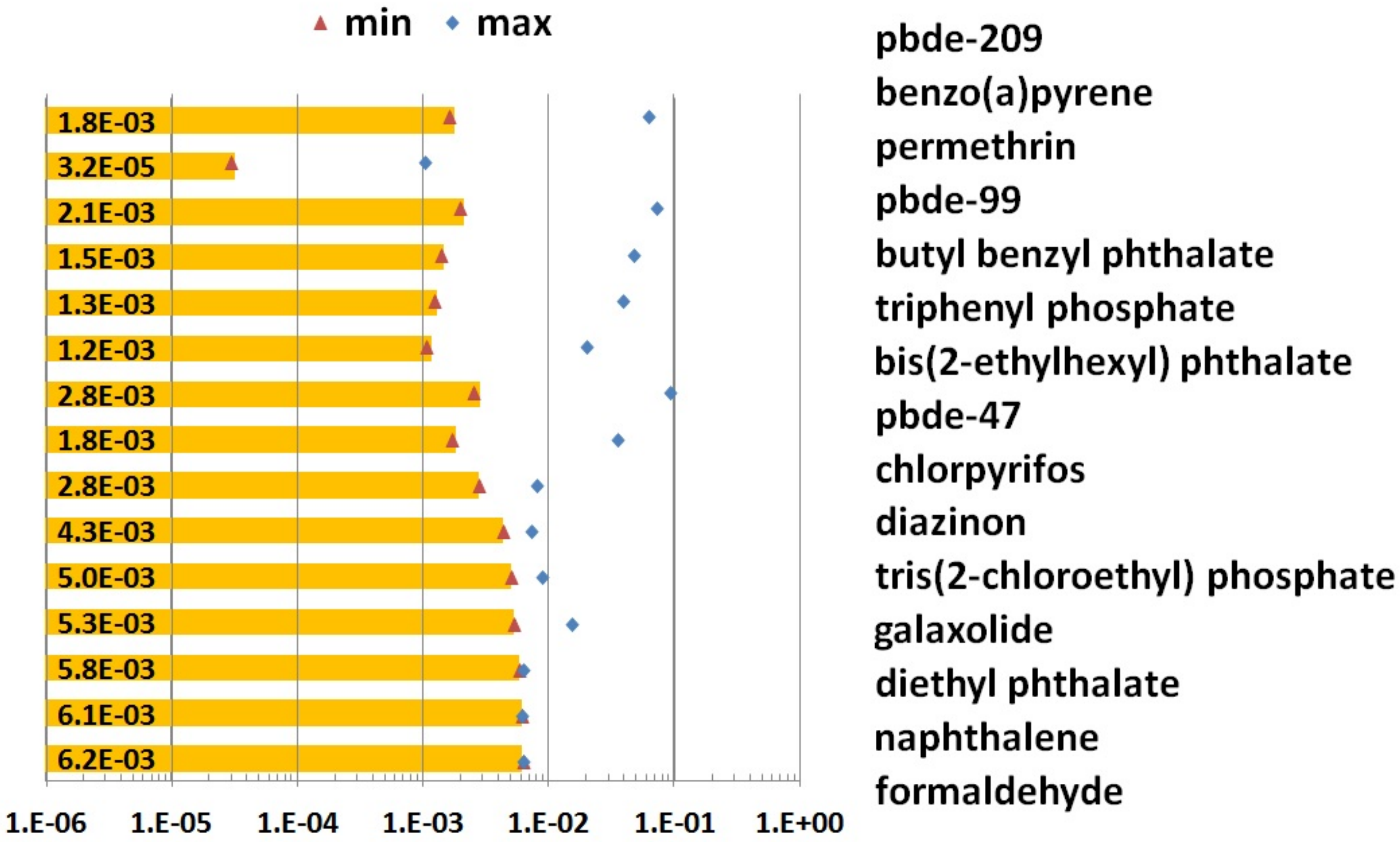
- **Correlated** with indoor air, other indoor surfaces, biological samples
- Known to be a **reservoir** for many compounds released indoors
- For SVOCs with low VP and high Koa, favorably **partition to dust**
  - More likely to have levels that exceed LOD and be analytically quantified
- Models are well developed that consider partitioning in various compartments in the home, from which we can **estimate exposure** through multiple routes





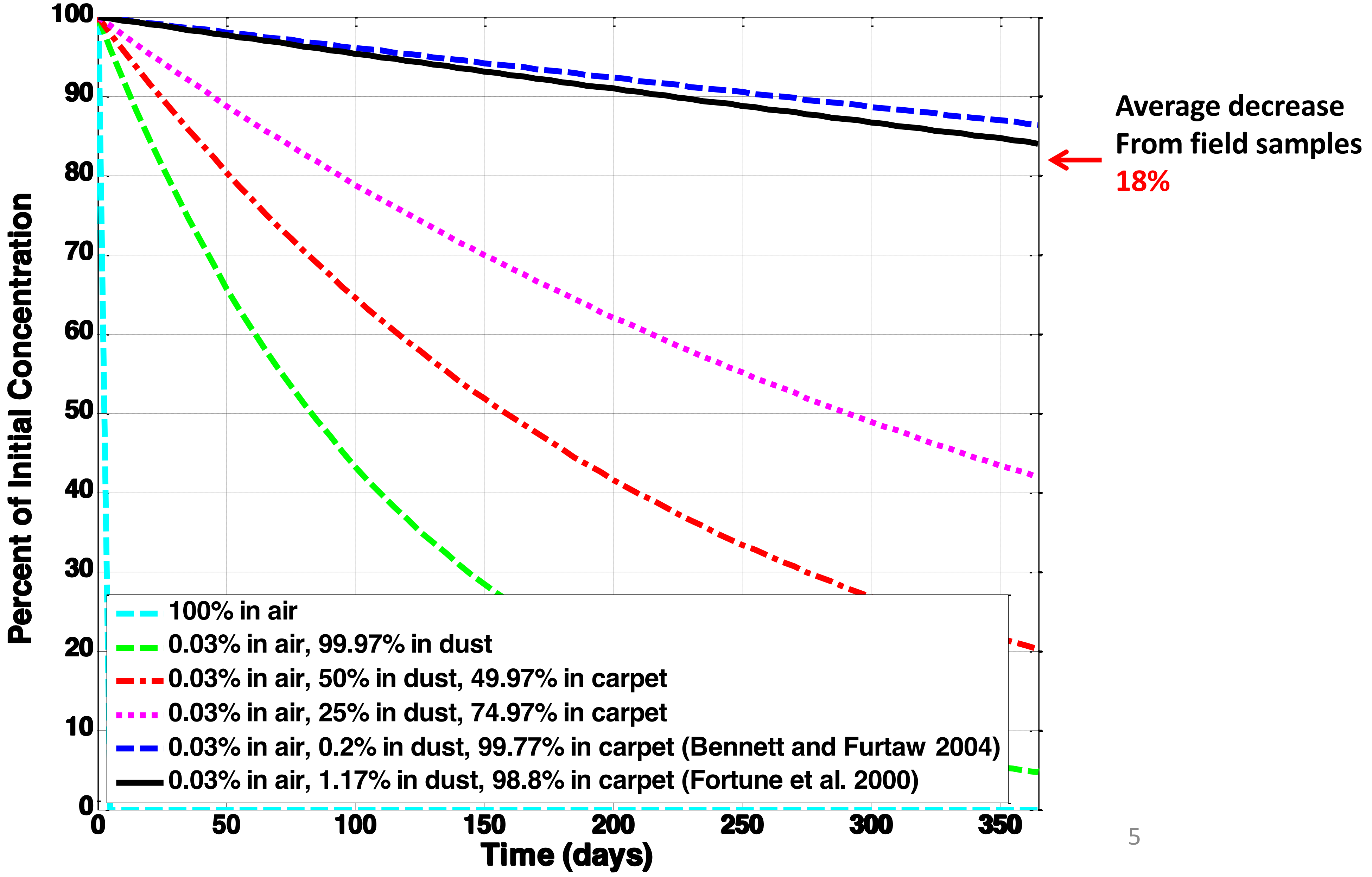
- Calculated intake fraction, assumed application to carpet
- Used multiple models for dermal uptake and non-dietary ingestion
- Potentially higher exposure per unit release than for volatile compounds

Indoor Intake Fraction



The more chemical in dust and surfaces, the longer the residence time

- Collected chlorpyrifos using passive air sampler 1 year apart in California in **2008** and **2009** from 38 homes
- Chlorpyrifos has not been sold for indoor use since **2001**
- **26 homes** decreased in concentration
- Evaluate modeled concentration changes by comparing with the annual average decrease



Calculating indoor exposures

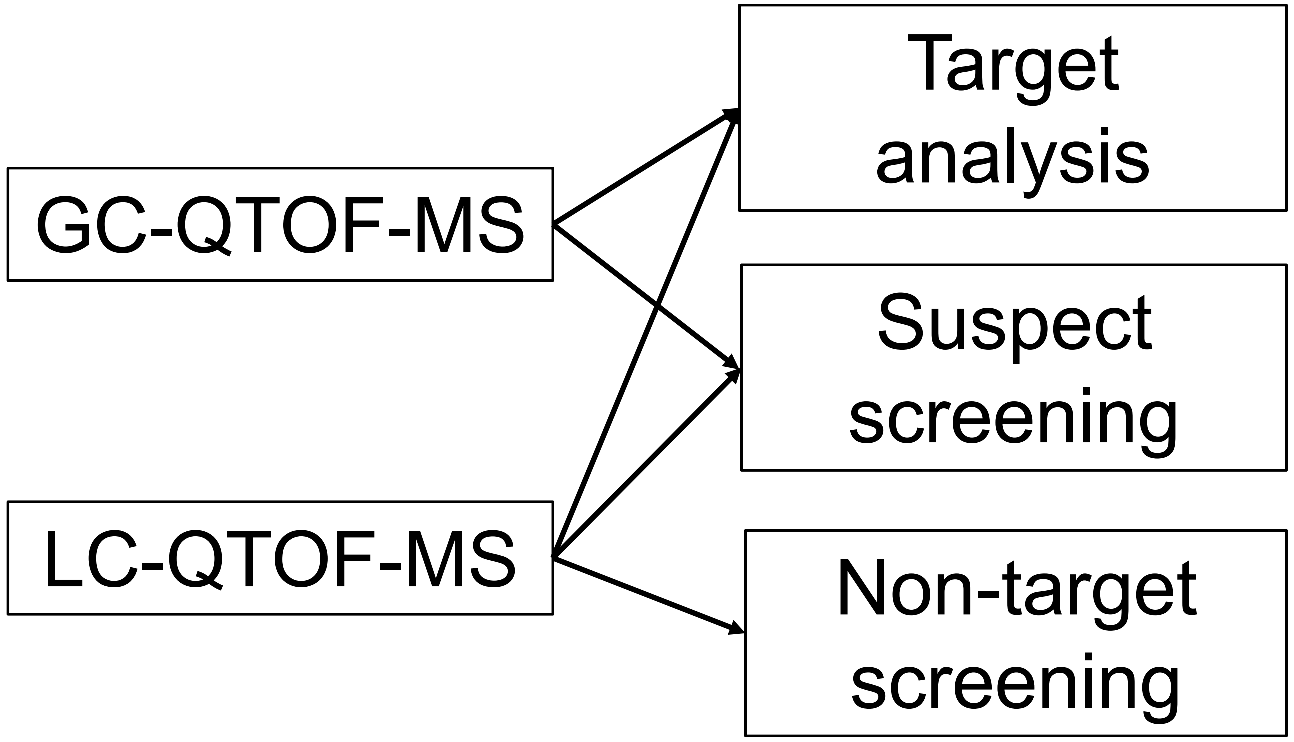
- Both sources and exposure models are equally important
- Many of the compounds we are concerned about in consumer products are SVOCs
- Emissions hard to estimate due to the lack of information
  - Chemical quantity introduced to each home (e.g., number of products containing chemicals of interest, chemical fraction in a product)
  - Use patterns (e.g., how the product is used, how often it is used)
  - Transfer mechanisms (e.g., how and how much chemicals are released or transferred from the products to indoor environments)

Instead, measure what is in dust

- Identify a broader range of compounds in dust to improve our understanding of potential sources
- Dust was Investigated by both LC-MS and GC-MS analytical platforms with three analytical approaches, target, suspect screening, and non-target
- Consider results in the context of consumer products and potential toxicity

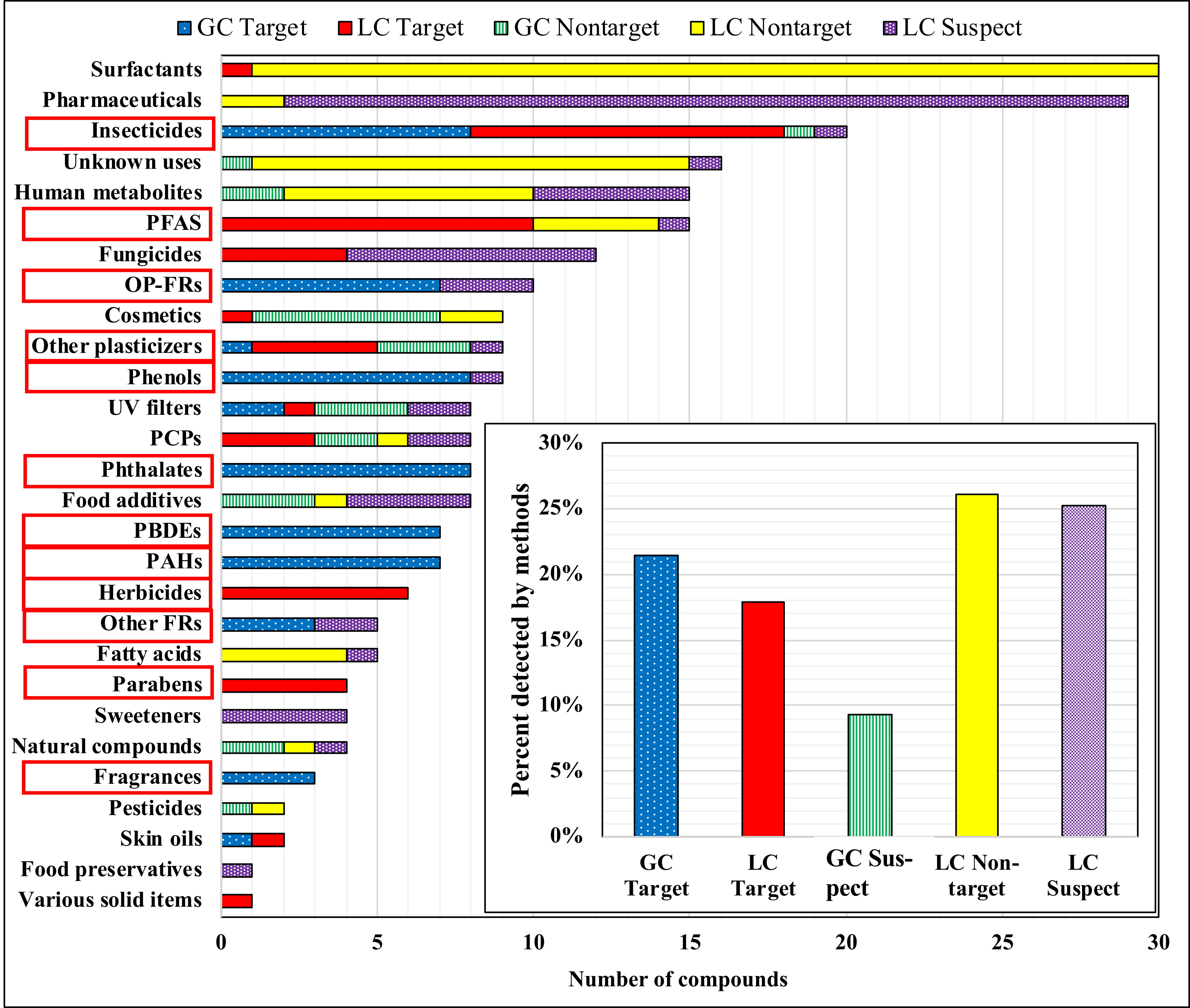
Sample collection and analysis

- Dust samples were collected using a high-volume small surface sampler (HVS3) from the main living area of **38** homes in Northern California (2015-2016)
- Analyzed *known* chemical classes → target
- Now include *expected* compounds using existing databases or libraries → suspect screening
- Also identify previously *unknown* compounds through high-resolution mass spec → non-target
- Standards purchased to confirm identity of suspect and non-targeted



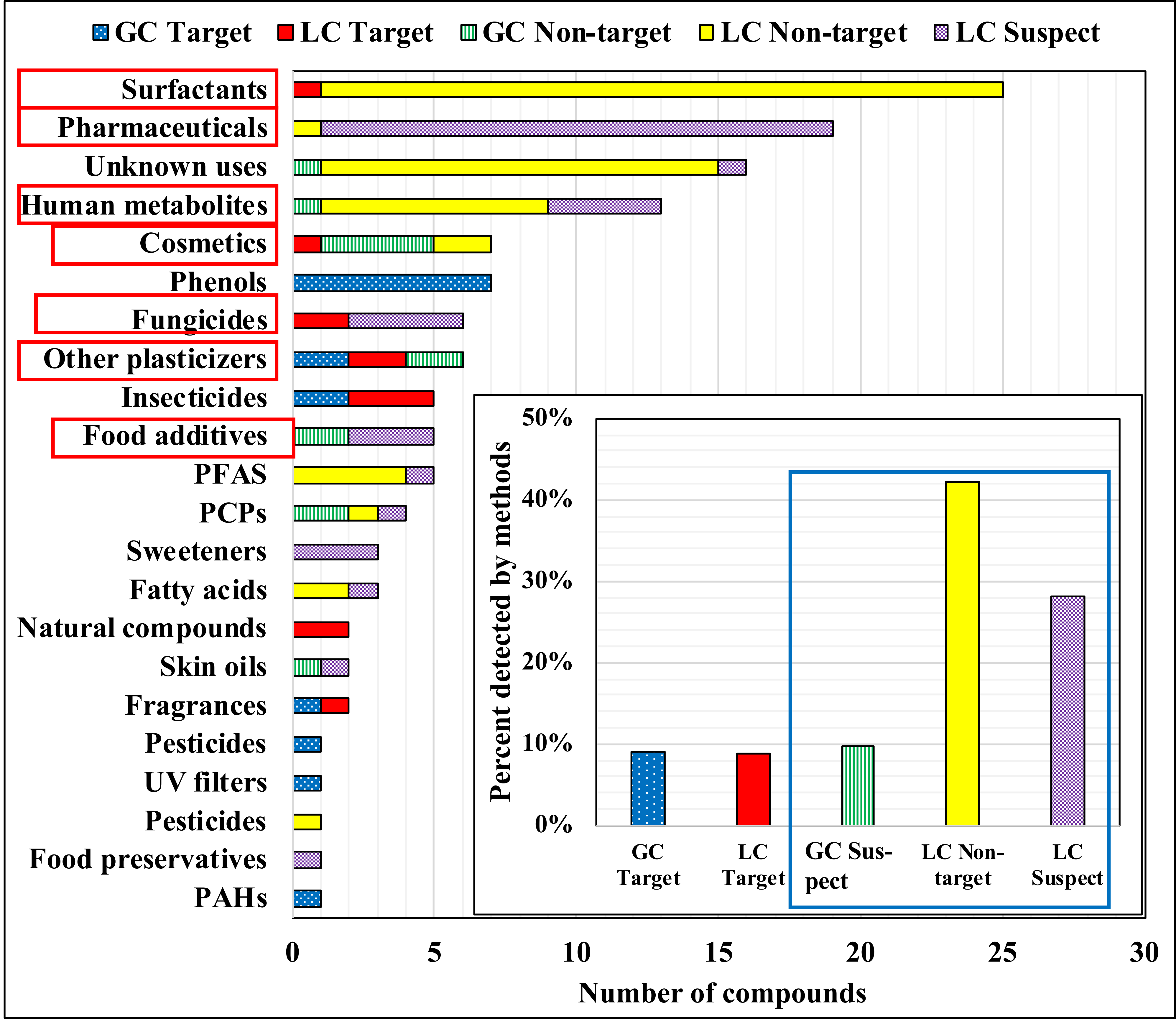
In total, 257 compounds detected

- Traditional compound classes identified via target methods



Of these, 135 were newly-measured compounds

- **81%** from GC suspect, LC suspect and LC non-target
- GC suspect screening found many cosmetic ingredients and other plasticizers
- LC suspect screening found many pharmaceuticals, fungicides, and food additives
- True non-target found many surfactants and human metabolites

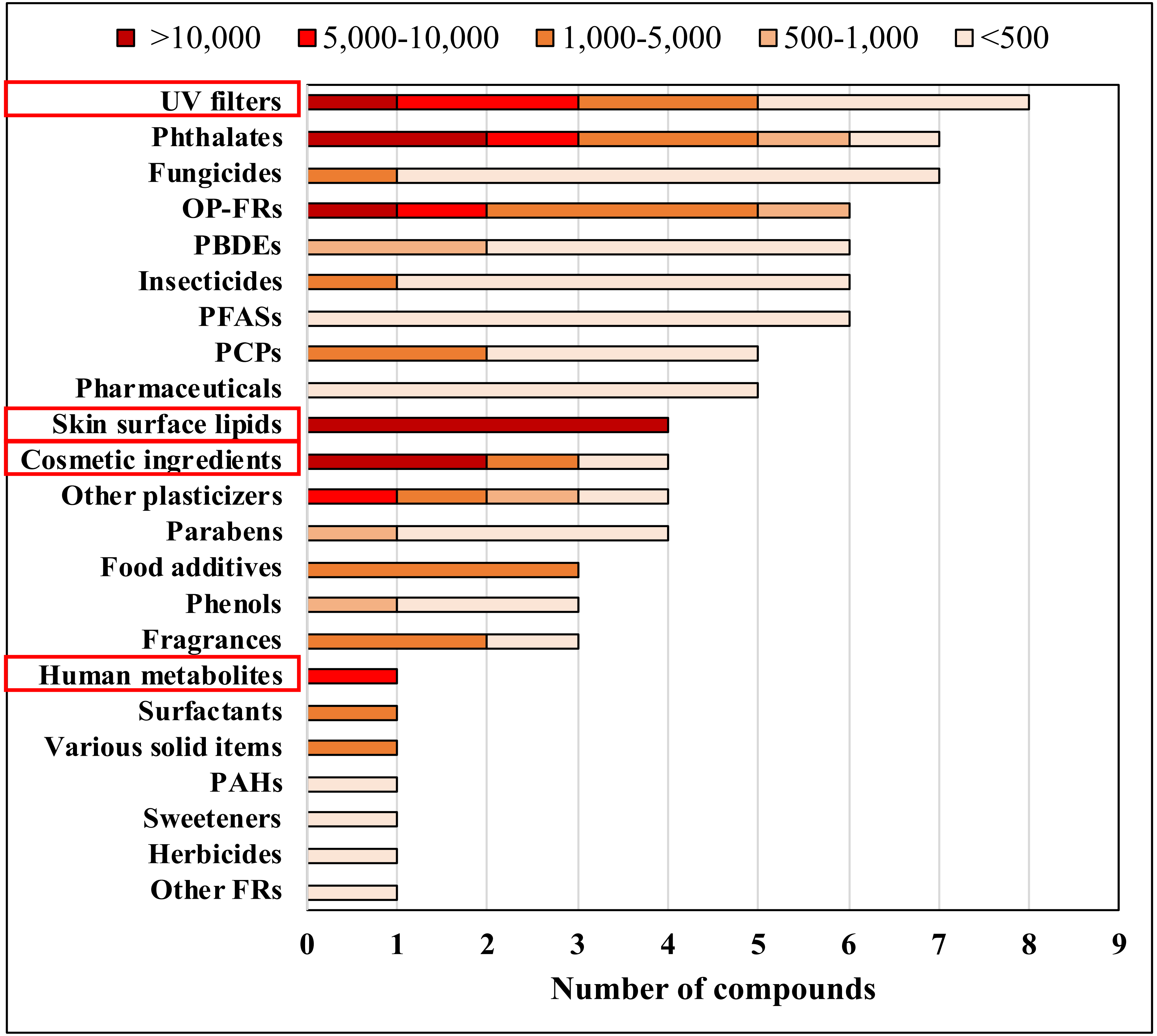


Relevance to consumer products

- Cosmetic ingredients – likely in dust due to skin flakes, and dust gives us a good way to access what compounds may be in products used in homes
- Alternative Plasticizers - Three compounds not previously measured in dust were near ubiquitous, indicates how quickly markets shift
- Fungicides – Compounds applied to fruit were frequently detected indoors
- Industrial Compounds – Ingredients of coatings and rubber widely detected in dust

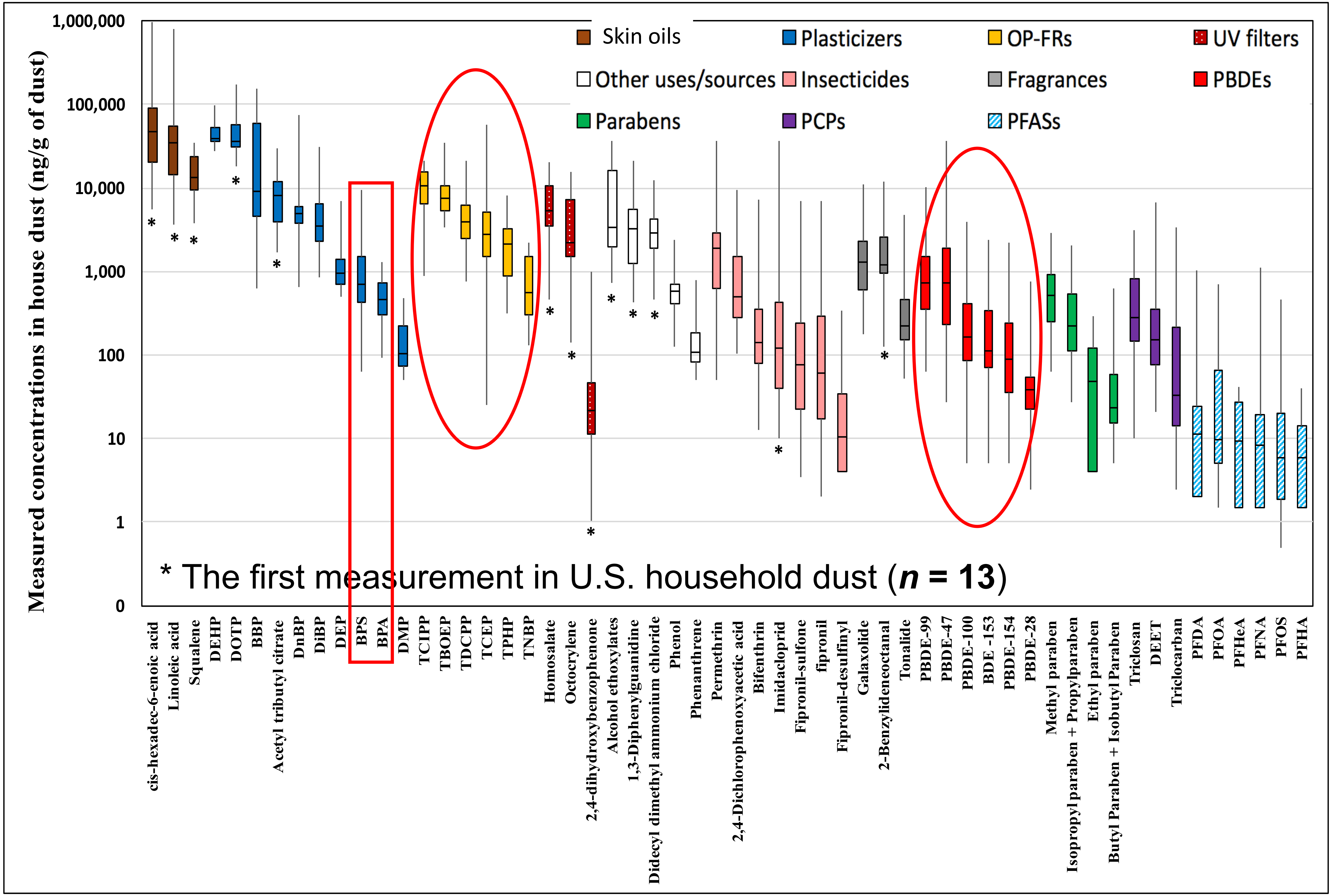
Median conc. (ng/g of dust) for **88** compounds detected in more than **50%** of samples

- Compound classes w/ high concentrations: humans and their activities, and possibly pets, play as sources of SVOCs in the indoor environment



Dust conc. for **56** target compounds detected in more than 50% of samples

Reflect recent changes in consumer use and changes in product formulation and regulations affecting PBDEs and BPA



in-vitro assays and models, primarily ToxCast

- **Neurological assays** – calcium, ligand, potassium, and sodium ion-channel assays directly from ToxCast Database. Integrated neural network activity assay
- **Endocrine Processes** - The four main processes were evaluated, estrogen, androgen, thyroid, and steroidogenic
  - Model with 18 *in vitro* HTS assays measuring estrogen receptor
  - model of 11 *in vitro* HTS assays measuring androgen receptor
  - Perturbed thyroid hormone homeostasis assays
  - Thyroid receptor activity
  - Model with multiple steroidogenic processes

Compounds with endocrine-disrupting or neurotoxic potential

- Utilizing results from *in vitro* high-throughput screening assays

257 compounds detected in our samples

65 compounds have endocrine-disrupting potential

- **28** pesticides
- **10** plasticizers
- **10** cosmetics/PCPs
- **4** flame retardants
- **3** PFAS
- **3** food sources (caffeine, sorbic acid, triethyl citrate)
- **7** other uses

29 compounds have neurotoxic potential

- **14** pesticides
- **4** plasticizers
- **4** cosmetics/PCPs
- **3** flame retardants
- **3** other uses

Compounds with endocrine-disrupting or neurotoxic potential

- Among **135** newly-detected compounds in our samples

17 compounds have endocrine-disrupting potential

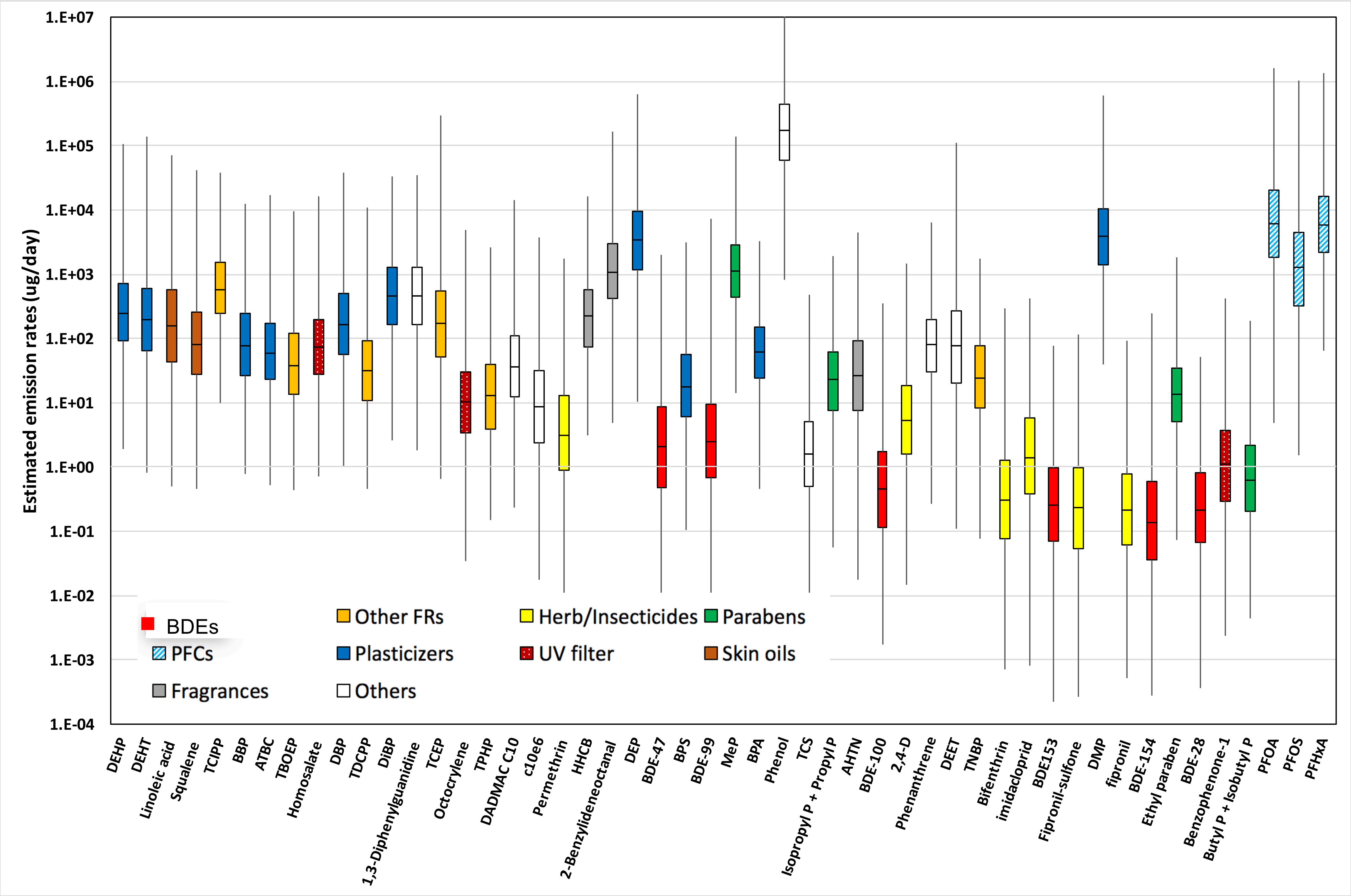
- **8** pesticides (**didecyldimethylammonium, fludioxonil, propiconazole, azoxystrobin, difenoconazole**, novaluron, methoxyfenozide carbendazim)
- **2** plasticizers (acetyl tributyl citrate; ATBC, dioctyl terephthalate; DOTP)
- **2** cosmetics/PCPs (2-benzylideneoctanal, benzyl benzoate)
- **2** food additives/preservatives (caffeine, sorbic acid)
- **3** other uses (**1,3-diphenylguanidine**, 2-chlorophenol, perfluoroundecanoic acid)

7 compounds have neurotoxic potential

- **6** pesticides (**didecyldimethylammonium, fludioxonil, propiconazole, azoxystrobin, difenoconazole**, esfenvalerate)
- **1** other uses (**1,3-diphenylguanidine**)

Detected in all homes

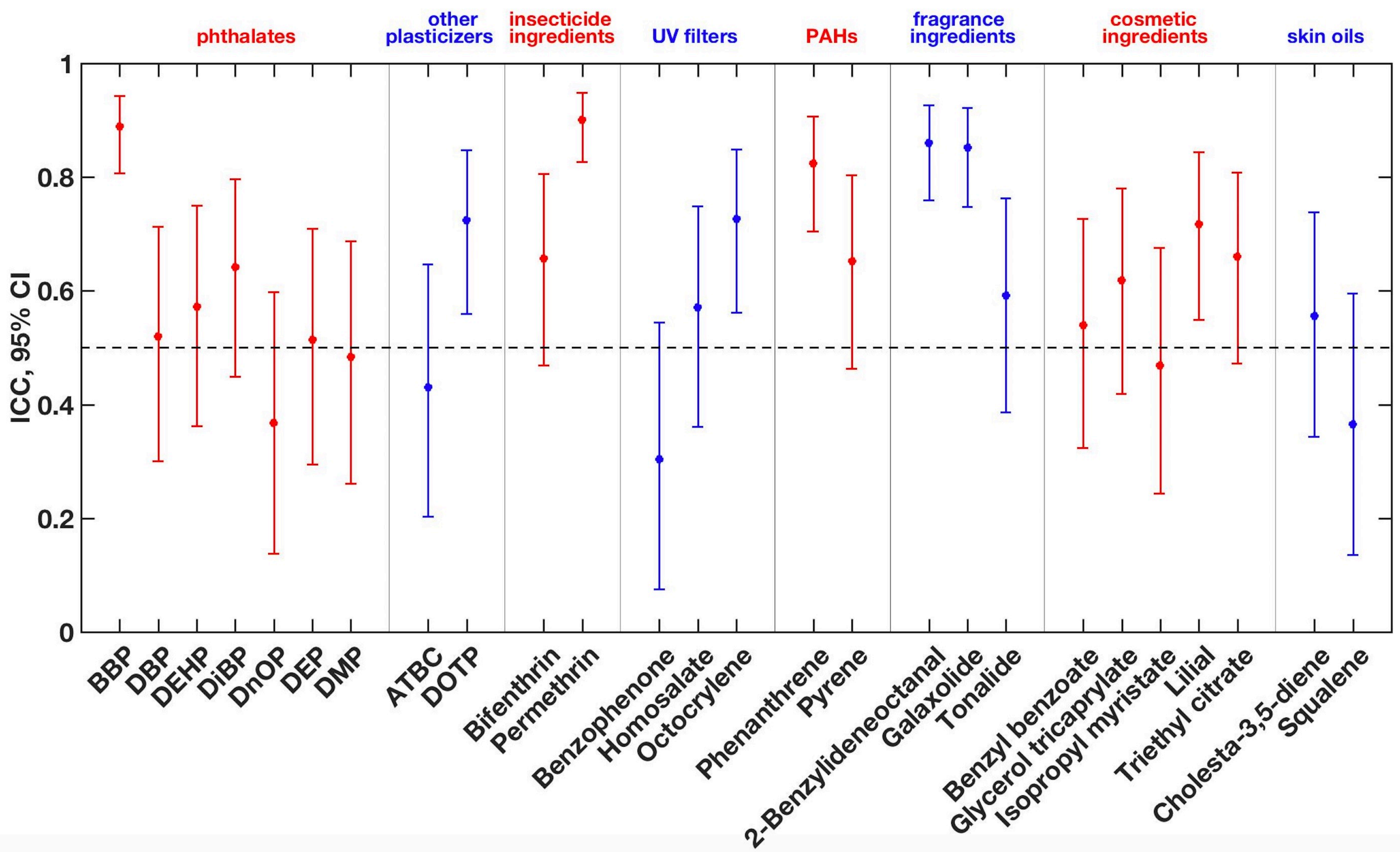
Estimated Emission Rates from Concentrations (ng/d)



Are dust concentrations measures of long term exposure?

- We care about changes in concentrations over time because if levels are consistent, it means people are exposed to these compounds over a long period of time
- A combination of persistence in the indoor environment and consistency of use patterns in the home

Levels in dust generally consistent

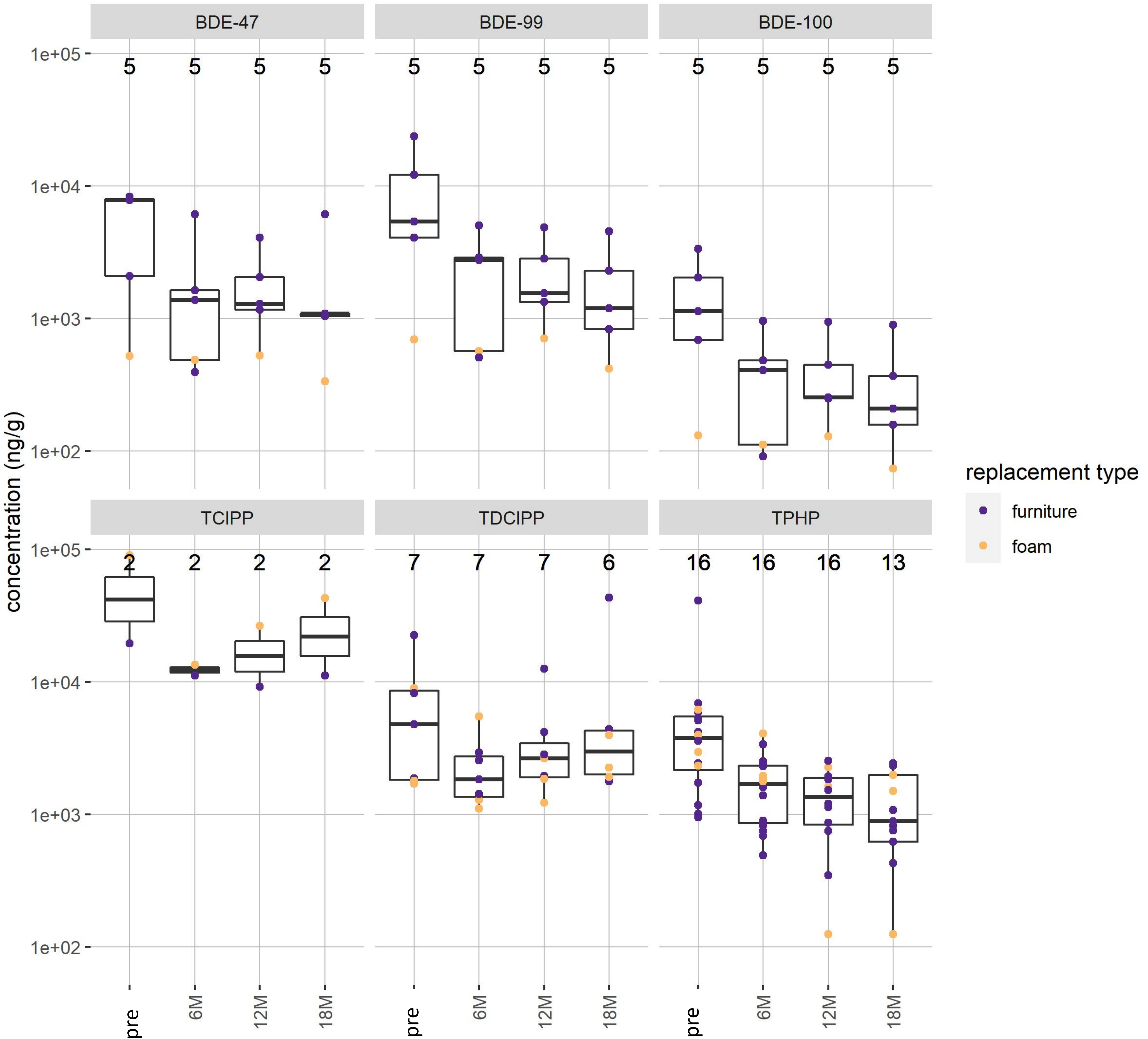


- Among 26 compounds detected in more than 50% of dust samples at all three visits, 20 compounds had ICCs above 0.50 and 6 compounds had ICCs below 0.50
- Overall, dust concentrations of insecticide ingredients, PAHs, and fragrance ingredients were more stable over time, with those of skin oils (or constituents of skin surface lipids) being the least stable

Replacing Furniture

When people removed furniture or replaced foam, indoor levels of what they removed went down

We should consider how to reduce indoor sources



Other Tools we can Utilize

- **E**nvironmental influences on **C**hild **H**ealth **O**utcomes (ECHO)
- Mapping Chemicals across Routes of Exposure and Body Burden: Data Gaps and Opportunities for ECHO
- Conducted a literature review to identify compounds with potential exposure and toxicity for which it seemed feasible to measure the compound in urine
- Developed a panel for urine analysis – Additional plasticizers, flame retardants, environmental phenols, aromatic amines, and pesticides
- First 100 samples from pregnant woman have been partially analyzed, with a larger sample being conducted soon
- Will allow us to identify other compounds with high exposure

Conclusions

- We need to continue to measure both dust and air, as well as bio-fluids, for a wide range of compounds to determine potential exposures
- High-throughput *in-vitro* assays and models can help us target our search
- The work EPA will be presenting next is another valuable tool for identifying other compounds we should be measuring
- While SVOCs have a long half-life indoors, we can make changes and see lower levels of exposure, and efforts should be made to identify other important sources that can be removed

Collaborators

- Hyeong-Moo Shin, Kyunghoon Kim - Univ. of Texas-Arlington
- Tom Young, Christoph Moschet, Rebecca Moran - UC Davis
- Tom McKone - UC Berkeley, LBNL
- Edo Pellazzari – Research Triangle Institute
- Jessie Buckley – John Hopkins University
- Kurunthachalam Kannon – New York University
- Robin Dotson, Kathryn Rodgers – Silent Spring Institute