Developing Chemical Signatures for Categories of Household Consumer Products Using Suspect Screening Analysis

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Introduction

- Consumer products are a major source of chemical exposure and therefore potential risk
- Knowing what combinations of chemicals are typically present in different types of products is needed for risk evaluation
- Quantifying similarity and variability of existing products can help in assessing new products and identifying uncommon chemical ingredients

Methods.

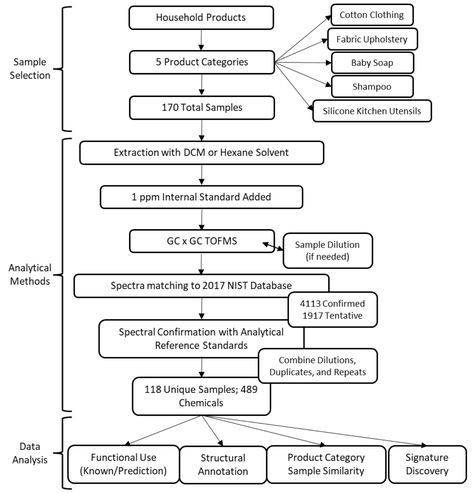


Figure 1. Suspect screening analysis (SSA) workflow for 5 types of household consumer products. Products were extracted with dichloromethane (DCM). Each extraction was analyzed via GCxGC-TOFMS to obtain its mass spectra. Spectra were matched to the 2017 NIST database. Analytical standards were used to confirm a subset of chemicals. Chemicals were annotated by functional uses and structural classification (ClassyFire).

Results

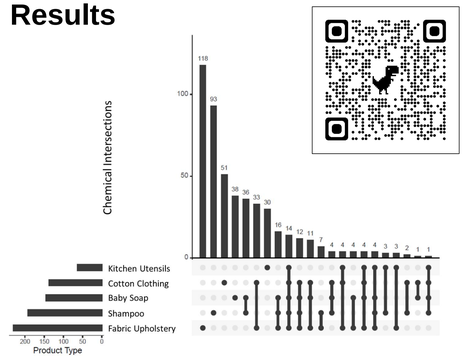
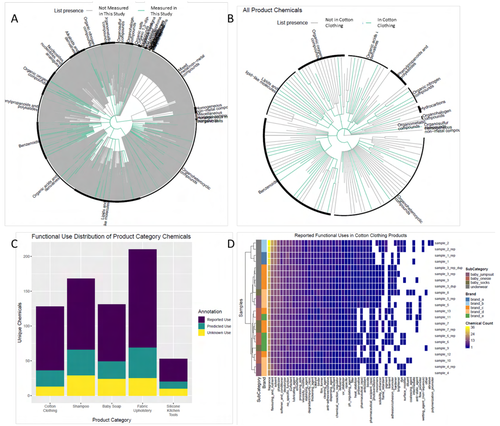


Figure 2. Upset plot showing how chemicals occurring in each of the five product categories intersect. The largest intersection is between baby soap and shampoo (36 shared chemicals). The left histogram shows the total number of unique chemicals measured across all samples in each product type, with fabric upholstery having the most.



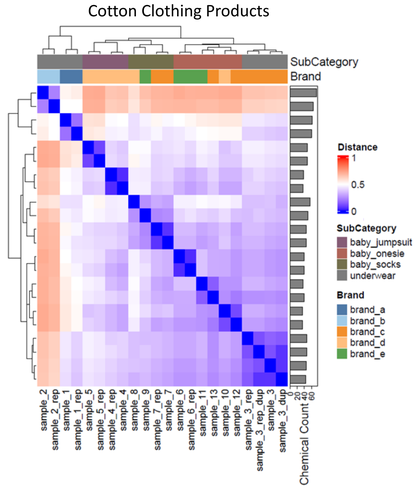


Figure 4. Sample similarity heatmap for all cotton clothing samples based on chemical occurrence. The Jaccard distance (0 = identical ingredients, 1 = no shared chemicals) was used to calculate sample similarity and cluster samples hierarchically. Anonymized product brand and category subtype are also indicated. "_rep" samples indicate a repeat purchase (two identical products) and "_dup" samples indicate two aliquots from the same individual product.

Figure 3. Annotation of chemicals identified by SSA. **A**. Chemical space spanned by all chemicals from all samples (green) within the full ClassyFire ChemOnt tree. **B**. Chemicals space spanned by cotton clothing-specific chemicals (green) within the tree spanned by chemicals in all samples. **C**. Functional use annotation distribution for the unique chemicals in each category. Predicted use indicates a QSUR model prediction with probability ≥ 80%. Unknown use indicates a prediction < 80% and/or outside the applicability domain. **D**. Count of reported chemical functions only in each cotton clothing sample. Samples are clustered by similarity.

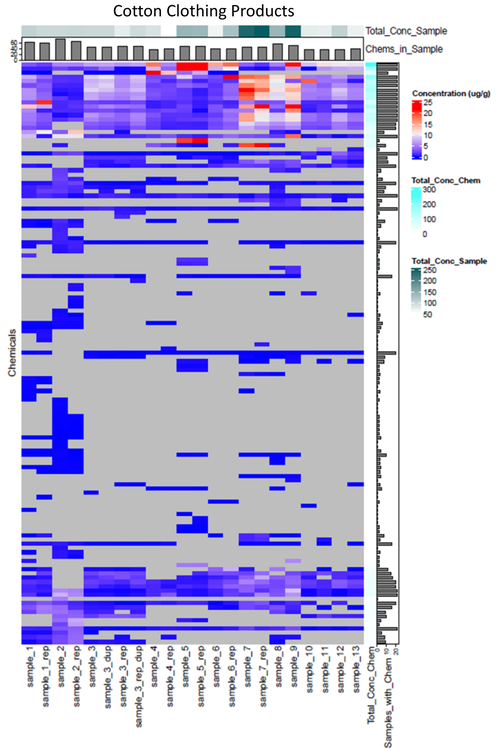


Figure 5. Heatmap of all chemicals identified in cotton clothing product samples. Reported sample abundances, total abundance across samples (top color bar) and chemicals (right color bar), and sample chemical counts (top bar plot) and chemical sample counts (right bar plot) are also shown. Rows (chemicals) are clustered hierarchically using the Euclidean distance.

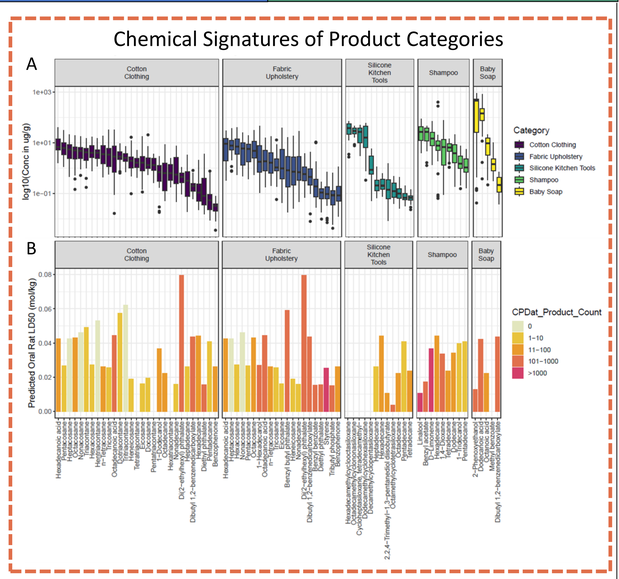


Figure 6. Chemical signatures for each product category. Chemicals were included in a signature if they occurred in ≥ 80% of product category samples. **A**. Reported abundance ranges, sorted from highest to lowest, based on the category samples in which each chemical was present. **B**. T.E.S.T. predicted oral rat LD50s in mol/kg for each signature chemical. Color indicates the number of products in CPDat (database containing product ingredient data reported by retailers and manufacturers) associated with each chemical. Chemicals without an associated bar in panel B had no available LD50 value.

Conclusions

- This study provides a baseline set of chemical ingredients (that is, representative mixtures) across common types of consumer products, which will aid in evaluating new and existing products.
- Separating constituent chemicals into typical and atypical can help inform exposure assessment, *in vitro* bioactivity screening, and ultimately the risk related to using such products.

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