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Chemical Characterization of Recycled Consumer Products Using Suspect Screening Analysis

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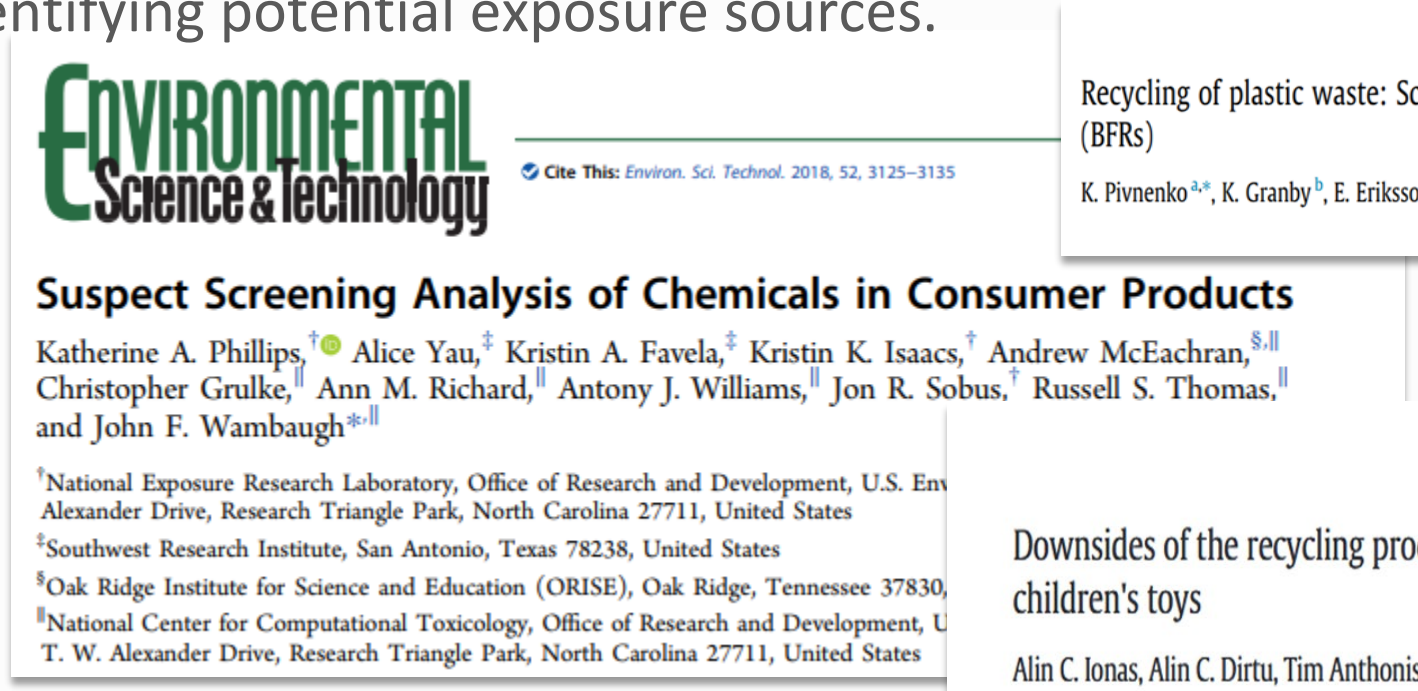
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Background

- The ExpoCast project seeks to rapidly understand and quantify chemical exposures across potential sources and pathways.
- Recycled consumer products may contain chemicals from source materials, contamination, or processing.
- Recycled and virgin materials are analyzed to characterize products and develop methods for identifying potential exposure sources.







Product categories



Construction materials



Fabric-containing consumer goods



Paper products



Children's toys and playmats



Food contact materials

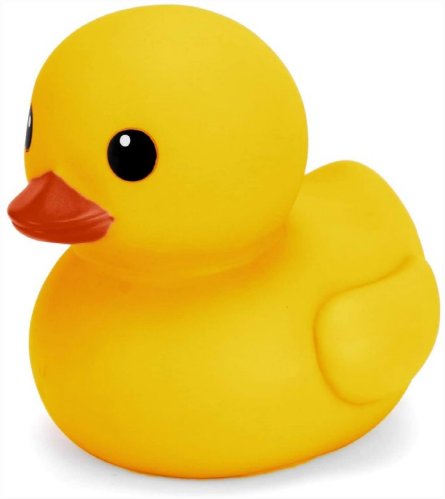


Plastic-containing consumer goods

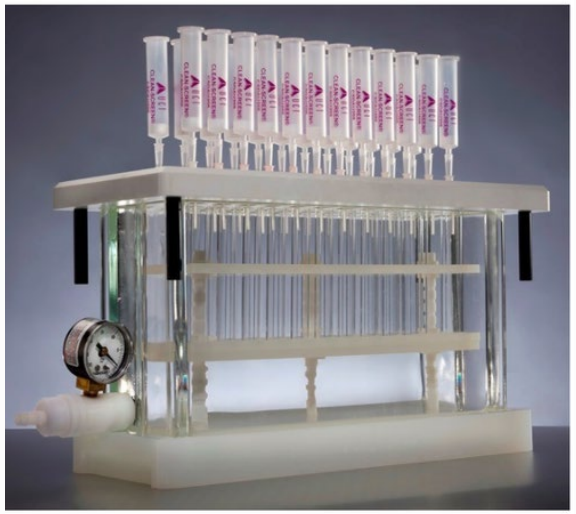


Products derived from recycled tire rubber

Suspect screening analysis



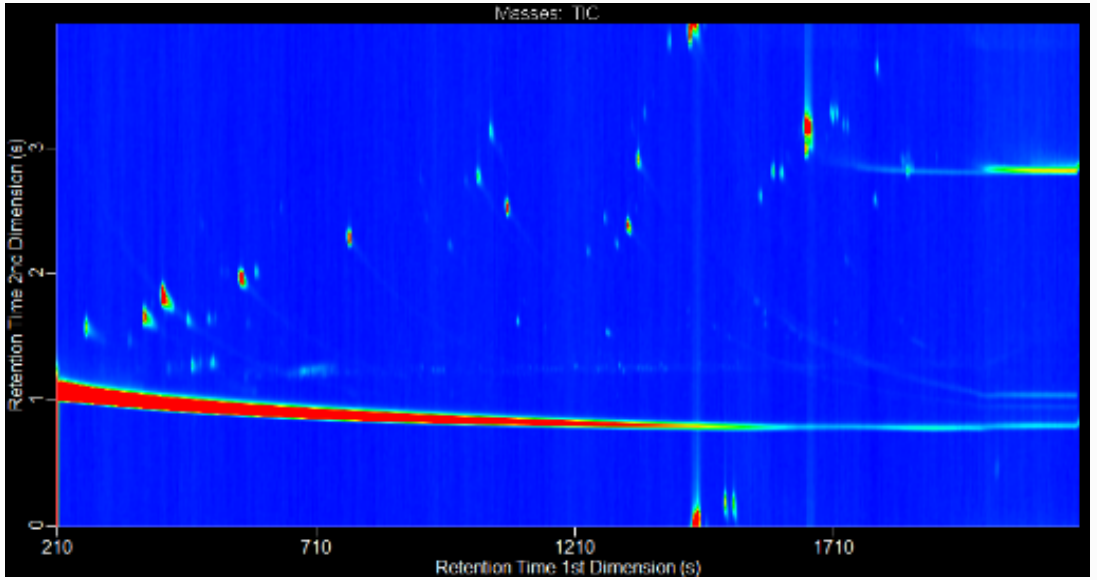
Media Sample



Extraction, Cleanup & Sample Preparation

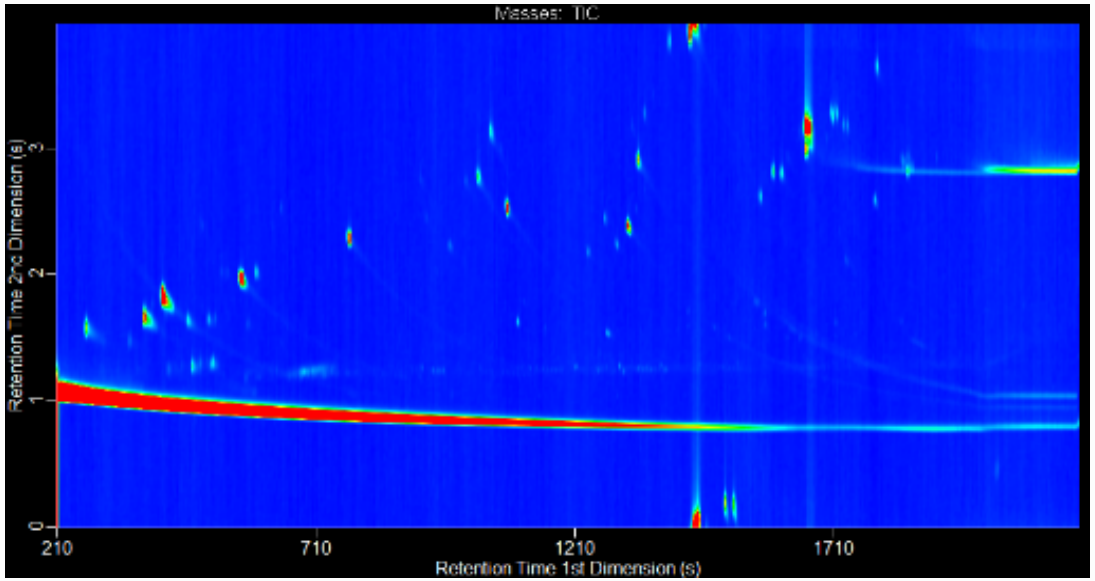


GC-MS Analysis

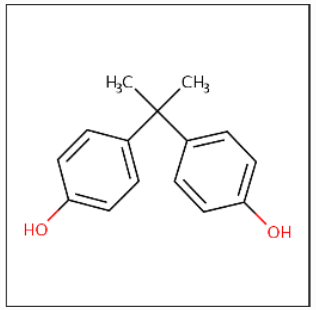


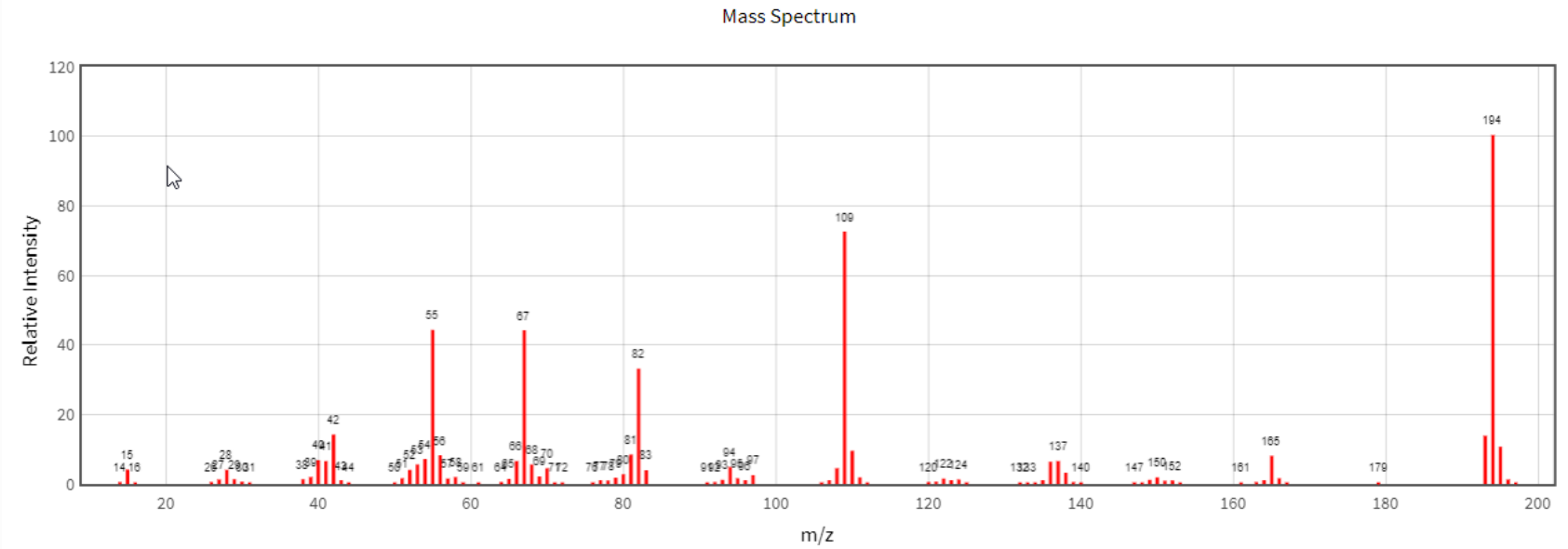
Suspect screening analysis

chemical identifiers
functional use(s)

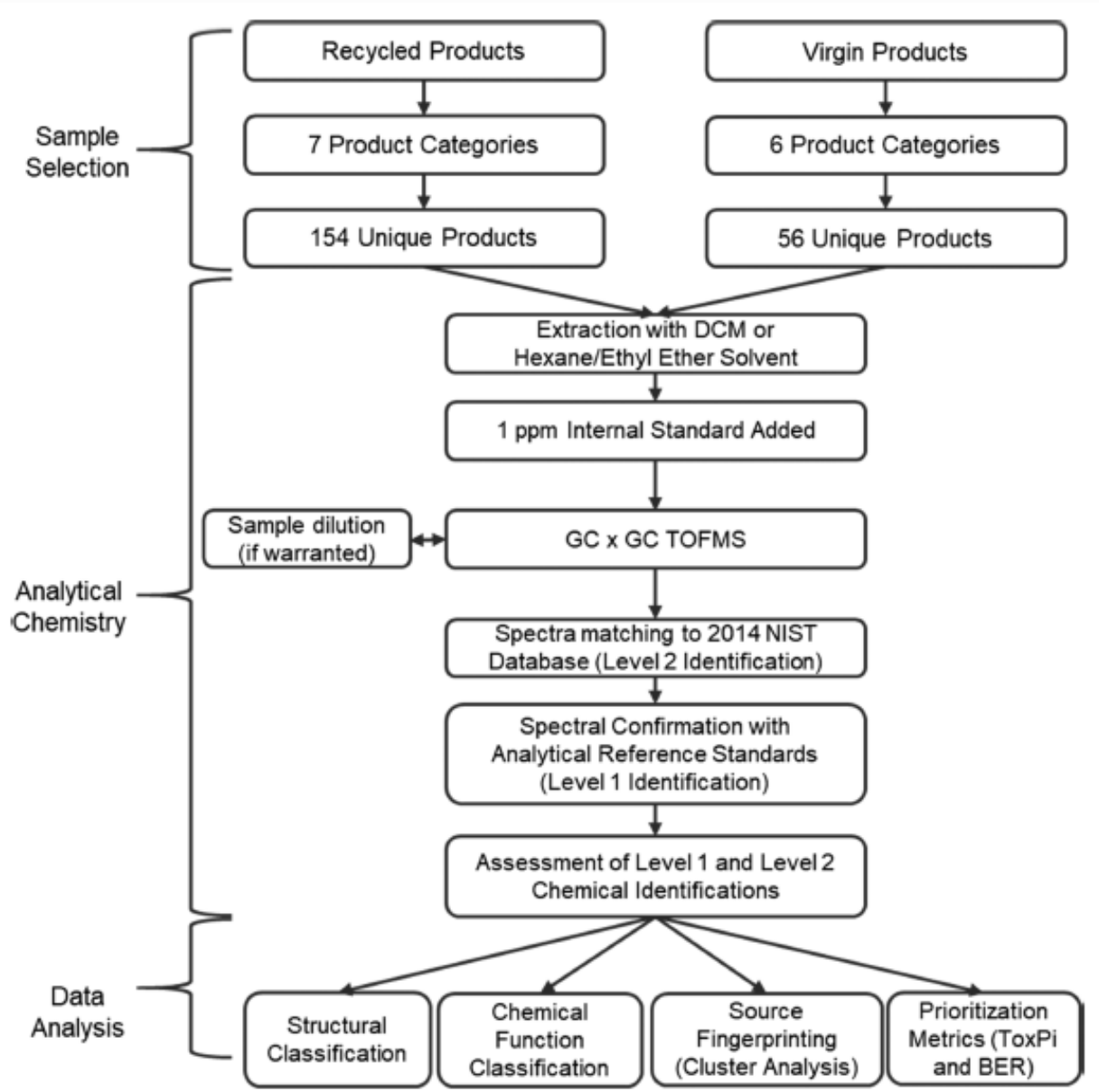


1000s of spectra





Workflow of product categorization and SSA



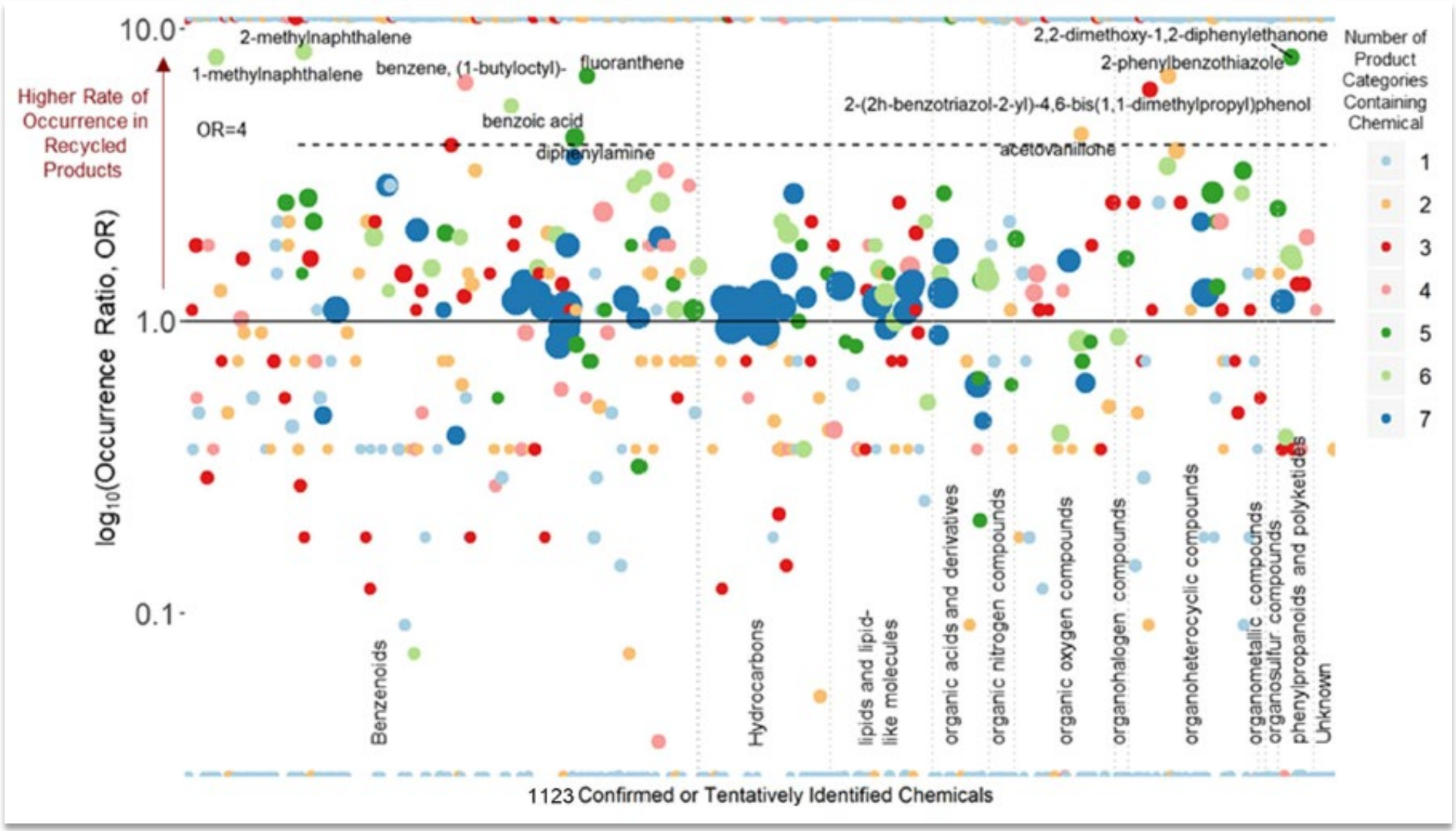
Number of level 1 & 2 chemicals per sample in product categories

category	$N_{recycled}$	$mean_{recycled}$	$median_{recycled}$	N_{virgin}	$mean_{virgin}$	$median_{virgin}$	*p*-value
all products	154	67.0	63	56	59.3	55	0.017
paper products	23	96.6	86	8	71.5	66.5	0.041
children's products	20	59.8	53.5	15	68.1	57	0.828
fabric products	17	82.4	89	14	64.1	63	0.242
recycled tire products	22	66.5	66.5				
food contact materials	22	59.9	60	11	56.6	54	0.417
construction materials	35	54.9	55	8	46.0	46.5	0.028
plastic home/auto products	15	53.5	55	20	49.2	36.5	0.054

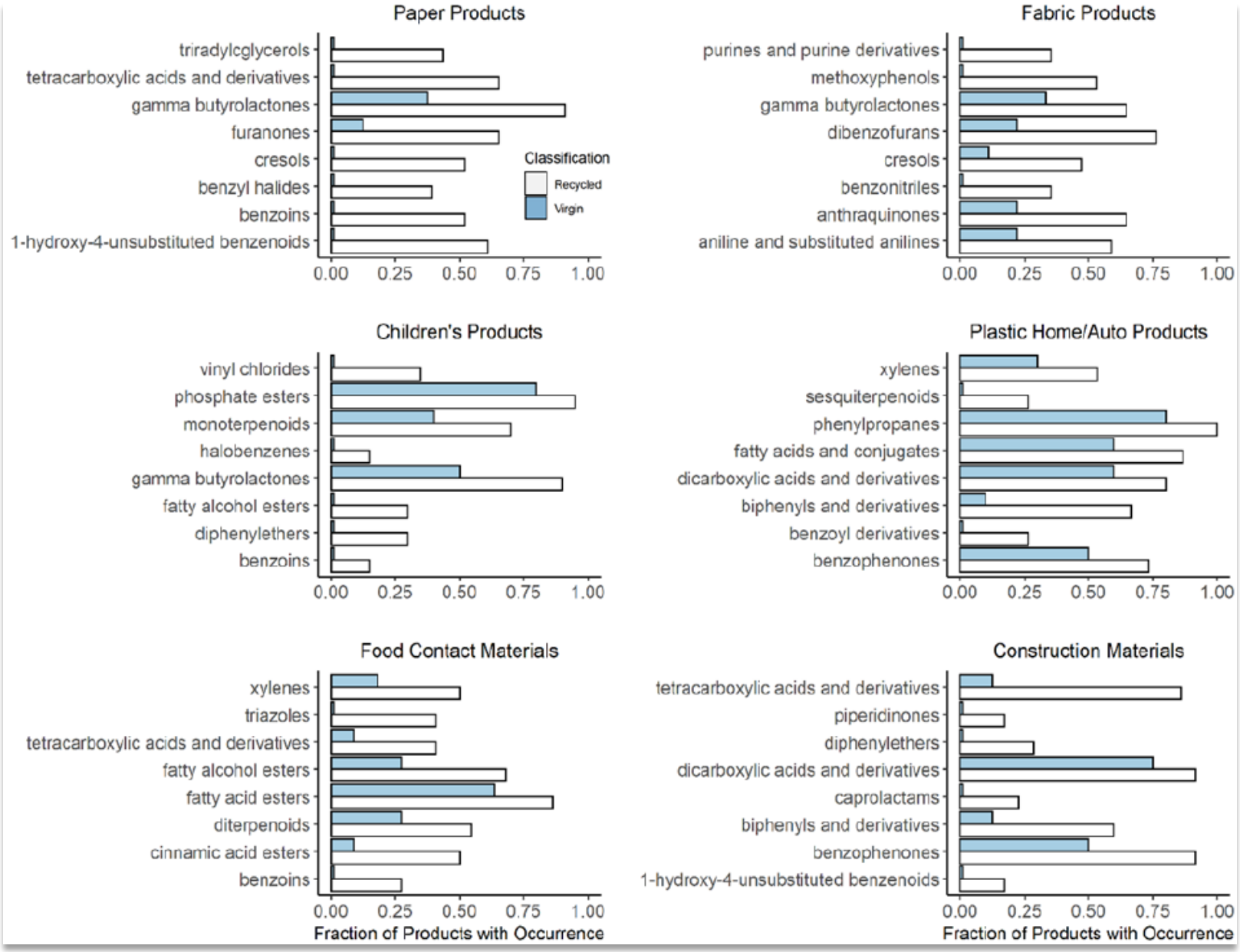
[a] $N_{recycled}$ and N_{virgin} refer to the number of recycled and virgin products that were tested.

- *Significantly* larger number of chemicals in recycled products less likely to be regulated/scrutinized versus virgin products.
- Categories more likely to be regulated (toys, food contact materials) contain statistically similar counts of chemicals in both recycled and virgin products.

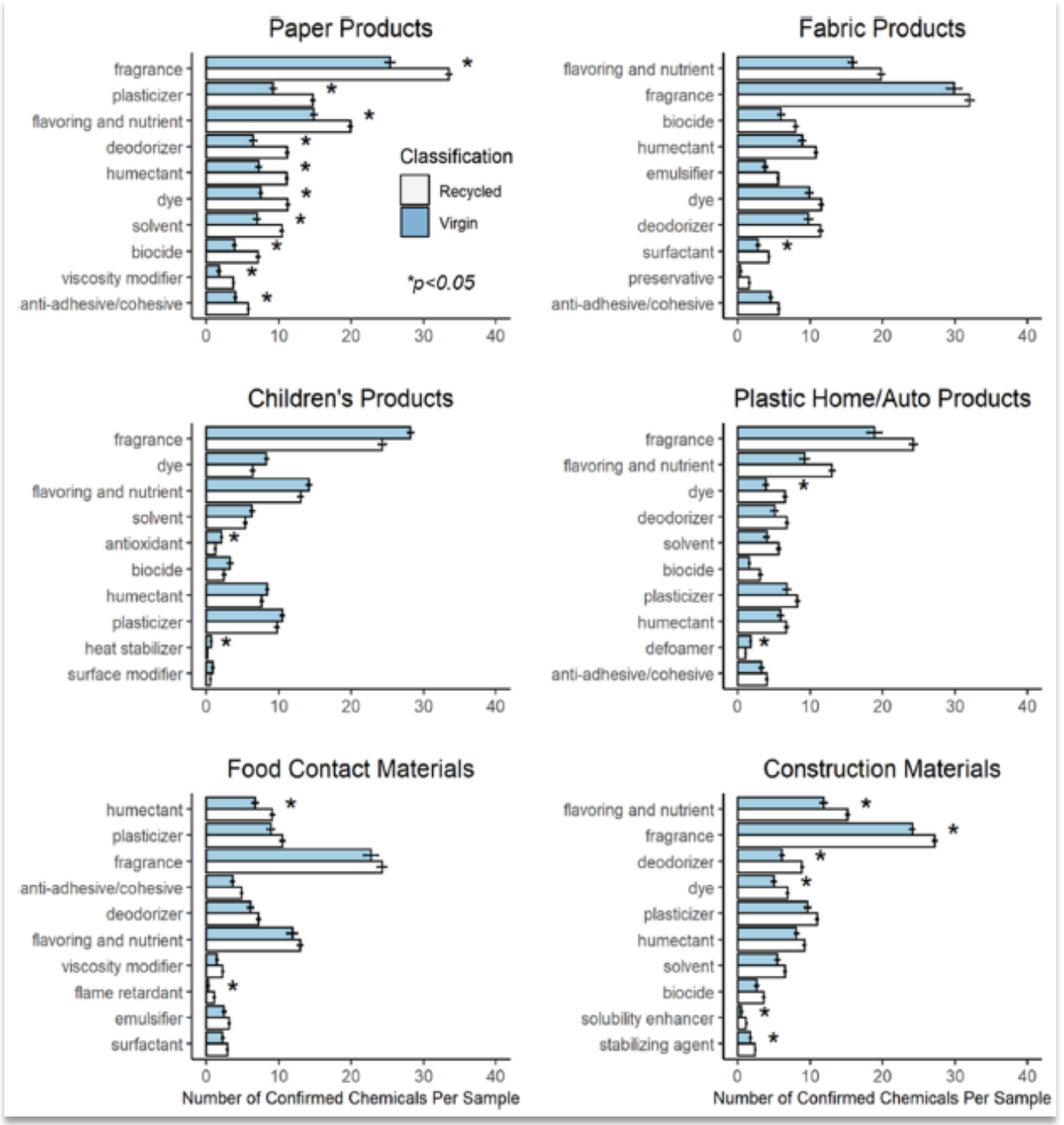
Occurrence ratios for 1,123 level 1 & 2 chemicals



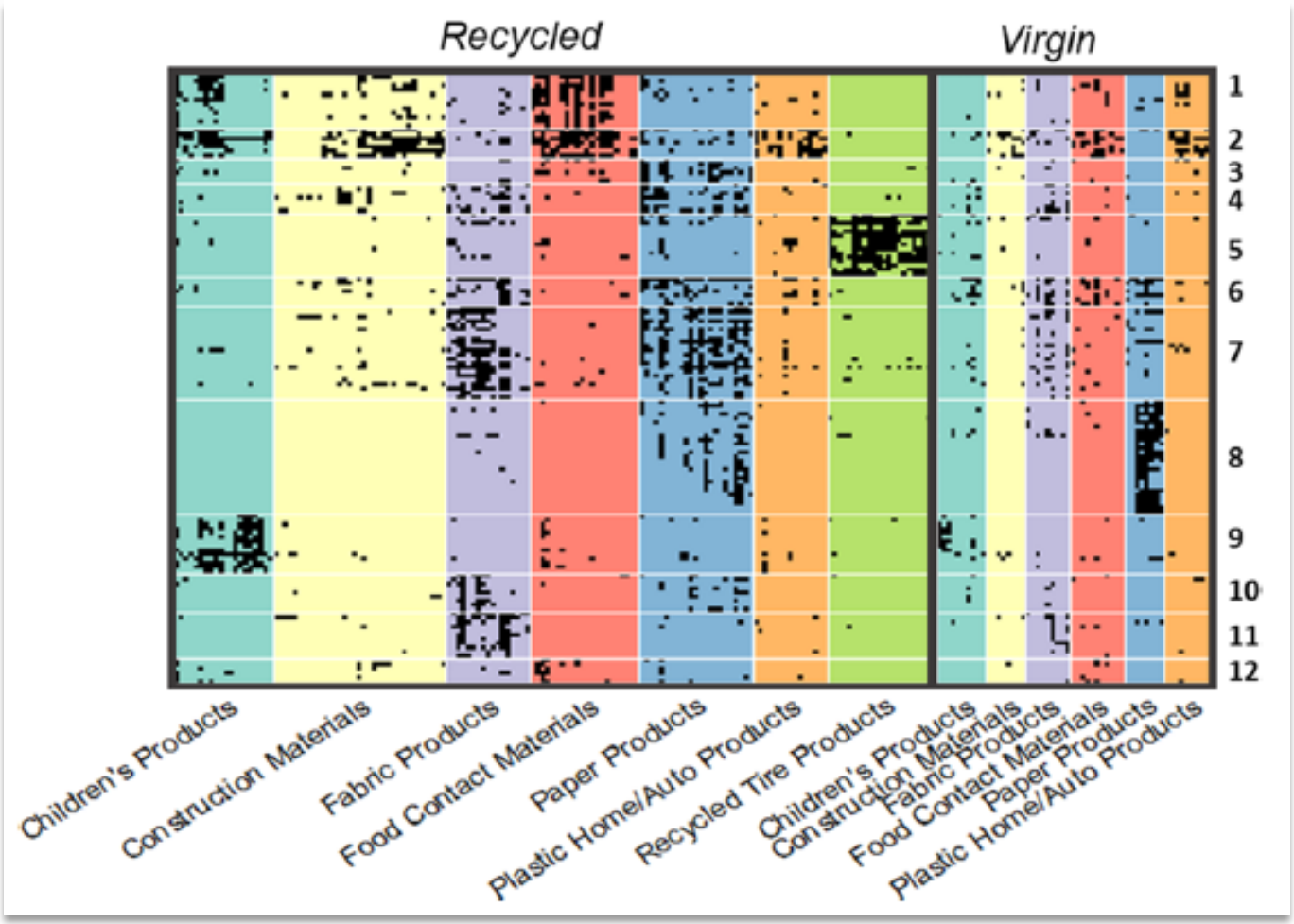
ClassyFire subclass categorization of chemicals



Functional Uses of confirmed chemicals



Clusters of level 1 & 2 chemicals in products



Clusters of particular interest

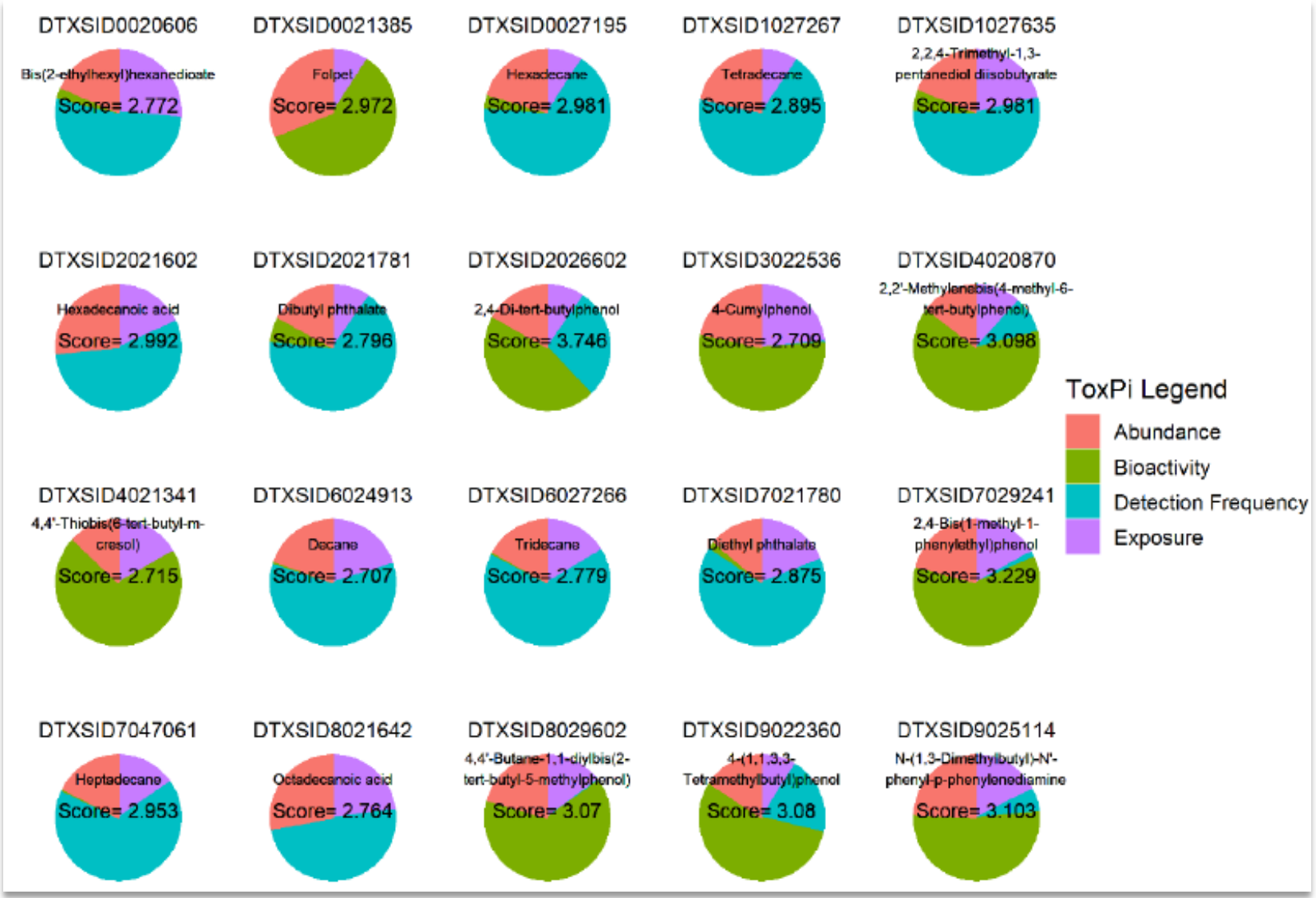
cluster ID	number of chemicals	primary classification	primary categories of occurrence[b]	frequently occurring uses, sectors, or functions[c]	example chemicals
1	13	recycled	children's products, construction products, food contact materials	pesticide actives and inerts	permethrin, bifenthrin, chlorpyriphos
2	7	both	children's products, construction materials, food contact materials, plastic home/auto products	plastics and plastics manufacturing (including intermediates), polymer additives (UV stabilizer, antioxidant, odor agent)	tris(2,4-di-*tert*-butylphenyl) phosphite, octadecyl 3-(3,5-di-*tert*-butyl-4-hydroxyphenyl)propionate, 2-(phenylmethylene) octanal
3	6	recycled	paper products	manufacture of ink, paints/coatings, or paper surface treatments; pesticides	2,2-dimethoxy-1,2-diphenylethanone, propylbenzene, DEET, *p,p'*-methoxychlor olefin
4	7	both	construction materials, fabric products, and paper products, fabric products	manufacture of ink, paints, or dyes; use in ink, toner, and colorant products	2-(2-butoxyethoxy)ethanol, (1-hydroxycyclohexyl)(phenyl) methanone, phthalic anhydride
5	15	recycled	recycled tire products	intermediates, rubber components, and processing aids used in the manufacture of rubber products or rubber tires, or in rubber recycling	aniline, diphenylamine, dicyclohexylamine, phthalimide
6	7	both	fabric and paper products, children's products, food contact materials	manufacture of plastics, including plasticizers or plasticizer precursors and other polymer additives.	triethyl citrate, dimethyl phthalate, benzaldehyde
7	22	both	paper products and fabric products	cleaning product, ink, and apparel manufacturing; solvents, fragrances, biocides, dyes, flame retardants	1-phenoxy-2-propanol, *p*-cresol, tris(2-chloroisopropyl) phosphate
8	27	both	paper products	dyes and dye manufacturing, fragrances, pigments and pigment manufacturing	leucomalachite green, Michler's ketone, dehydroabietic acid
9	14	both	children's products	an alternative plasticizer used in children's products due to its low toxicity; adhesives, colorants, and chemicals used in their production	bis(2-ethylhexyl) terephthalate, tetradecanoic acid, 1,4-bis(2-hydroxy-2-propyl)benzene
10	9	recycled	fabric and paper products	fragrances, flavorants, manufacturing of chemicals, cleaning and washing	methyl benzoate, triclosan, dimethyl succinate
11	11	both	fabric products	flame retardants, fragrances, apparel manufacturing	2-butyl-1*H*-isoindole-1,3(2*H*)-dione, octrizole, biphenyl phosphate
12	6	both	food contact materials	polymer additives (e.g., odor agent, stabilizers); intermediates	2-hydroxy-4-methoxybenzophenone, hexyl salicylate, 3,5-di-*tert*-butyl-4-hydroxyhydocinnamic acid

Toxicological priority index (ToxPi)

$$ToxPi\ Score_i = w_A \frac{A_i - A_{min}}{A_{max} - A_{min}} + w_N \frac{N_i - N_{min}}{N_{max} - N_{min}} + w_E \frac{E_i - E_{min}}{E_{max} - E_{min}} + w_B \frac{B_i - B_{min}}{B_{max} - B_{min}}$$

- A: Relative abundance
- N: Detection frequency
- E: Exposure potential
- B: Bioactivity

14 of the 20 highest ToxPi scores have Occurrence ratios > 1



Limitations

- Occurrence of chemical does not necessarily imply exposure.
- Recycled products contain ≥ 50% recycled material.
- Only chemicals amenable to GC-MS and found in the NIST 2014 library are identified.
- Semivolatile chemicals (e.g., benzyl butyl phthalate, tris(2-ethylhexyl) phosphate) potentially firmly bound in product matrix.
- Low-resolution instrument used rather than a high-resolution instrument

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Thank you for
Listening!