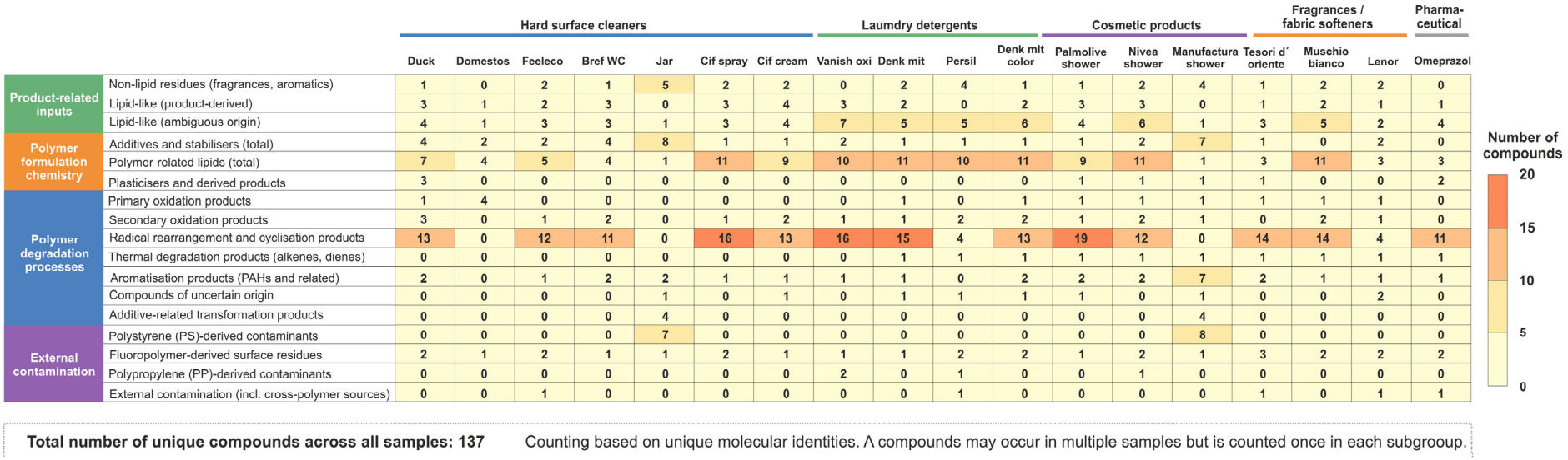
Supplementary material – Figure S1

Linking degradation pathways, additive transformation, and contaminant profiles in post-consumer HDPE: implications for recycling quality

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Supplementary Figure S1: Heatmap showing the distribution of compound subgroups across individual samples, based on the number of unique compounds in each subgroup.



		Hard surface cleaners							Laumdry detergents				Cosmetic products			Fragrances / fabric softeners			Pharma-ceutical
		Duck	Domestos	Feeleco	Bref WC	Jar	Cif spray	Cif cream	Vanish oxi	Denk mit	Persil	Denk mit color	Palmolive shower	Nivea shower	Manufactura shower	Tesori d´oriente	Muschio bianco	Lenor	Omeprazol
Product-related inputs	Non-lipid residues (fragrances, aromatics)	1	0	2	1	5	2	2	0	2	4	1	1	2	4	1	2	2	0
	Lipid-like (product-derived)	3	1	2	3	0	3	4	3	2	0	2	3	3	0	1	2	1	1
	Lipid-like (ambiguous origin)	4	1	3	3	1	3	4	7	5	5	6	4	6	1	3	5	2	4
Polymer formulation chemistry	Additives and stabilisers (total)	4	2	2	4	8	1	1	2	1	1	1	1	2	7	1	0	2	0
	Polymer-related lipids (total)	7	4	5	4	1	11	9	10	11	10	11	9	11	1	3	11	3	3
	Plasticisers and derived products	3	0	0	0	0	0	0	0	0	0	0	1	1	1	1	0	0	2
Polymer degradation processes	Primary oxidation products	1	4	0	0	0	0	0	0	1	0	1	1	1	1	1	1	1	0
	Secondary oxidation products	3	0	1	2	0	1	2	1	1	2	2	1	2	1	0	2	1	0
	Radical rearrangement and cyclisation products	13	0	12	11	0	16	13	16	15	4	13	19	12	0	14	14	4	11
	Thermal degradation products (alkenes, dienes)	0	0	0	0	0	0	0	0	1	1	1	1	1	1	1	1	1	1
	Aromatisation products (PAHs and related)	2	0	1	2	2	1	1	1	1	0	2	2	2	7	2	1	1	1
	Compounds of uncertain origin	0	0	0	0	1	0	1	0	1	1	1	1	0	1	0	0	2	0
	Additive-related transformation products	0	0	0	0	4	0	0	0	0	0	0	0	0	4	0	0	0	0
External contamination	Polystyrene (PS)-derived contaminants	0	0	0	0	7	0	0	0	0	0	0	0	0	8	0	0	0	0
	Fluoropolymer-derived surface residues	2	1	2	1	1	2	1	1	1	2	2	1	2	1	3	2	2	2
	Polypropylene (PP)-derived contaminants	0	0	0	0	0	0	0	2	0	1	0	0	1	0	0	0	0	0
	External contamination (incl. cross-polymer sources)	0	0	1	0	0	0	0	0	0	1	0	0	0	0	1	0	1	1

Total number of unique compounds across all samples: 137 Counting based on unique molecular identities. A compounds may occur in multiple samples but is counted once in each subgroup.