Supporting Information

For

Widespread Presence of Chlorinated Paraffins in Consumer Products

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This supporting information provides text and figures addressing (1) Method for semi-quantification of chlorinated paraffins; (2) Sampled products information; (3) Detection limits; (4) Recoveries; (5) Chlorine contents of CP technical mixtures; (6) Photos of consumer products with high concentrations of CPs; (7) Atomic distributions of CP Homologues in representative products.

Semi-Quantitation of Chlorinated Paraffins

Six technical mixtures of CPs were used for this method: 2 SCCP mixtures (C_{10}-C_{13}, 51.5% Cl; C_{10}-C_{13}, 63% Cl), 2 MCCP mixtures (C_{14}-C_{17}, 42% Cl; C_{14}-C_{17}, 57% Cl), and 2 LCCP mixtures (C_{18}-C_{20}, 36% Cl; C_{18}-C_{20}, 49% Cl). Quantification of CPs was based on the method of Reth et. al.[1] and is summarized by Eqs. 2-8 below.

For each technical mixture, peak areas of the most abundant isotope of each common $[M+Cl]^-$ Homologue were collected and normalized by the peak area of the mass-labelled internal standard $^{13}C_{10}$-anti-DP, which was added to every standard solution and spiked into every sample at the same concentration.

$$Normalized\ Isotope\ Area = \frac{Isotope\ Peak\ Area}{Internal\ Standard\ Peak\ Area} \quad (2)$$

The full area of each detected Homologue was then estimated by dividing the normalized area by the natural percent abundance of the isotope peak detected.

$$Normalized\ Congener\ Peak\ Area = \frac{Normalized\ Isotope\ Area}{\%\ Abundance\ of\ Detected\ Isotope} \quad (3)$$

The response factor (RF) for each technical mixture was calculated by dividing the sum of all Homologue peak areas in the mixture by the concentration used.

$$RF\ (Mixture) = \frac{\sum Normalized\ Congener\ Peak\ Areas}{Technical\ Mixture\ Concentration} \quad (4)$$

Chlorine content for the technical mixture was calculated from the exact mass % of chlorine for each Homologue using Eq. 5. As CP Homologues with fewer chlorines (<5) are more difficult to detect, this method often overestimates the chlorine contents of technical mixtures with

lower degrees of chlorination. Table S4 summarizes the difference between calculated and manufacturer-provided chlorine contents for each technical mixture used.

$$\%\ Cl\ (Mixture) = \sum\left(\frac{Normalized\ Congener\ Peak\ Area}{\sum Normalized\ Congener\ Peak\ Areas} * \%Cl\ (Congener)\right) \quad (5)$$

The exact mass % of chlorine for each Homologue was obtained using Eq. 6:

$$\%Cl\ (Congener) = \frac{Total\ Molar\ Mass\ of\ Cl\ in\ Congener}{Molecular\ Mass\ of\ Congener} \quad (6)$$

The RF was then plotted against the %Cl for each pair of mixtures containing the same CP chain lengths, and linear regression was performed to obtain three different versions of Eq. 7, one each for SCCPs, MCCPs, and LCCPs:

$$RF\ (Mixture) = a * \%Cl\ (Mixture) + b \quad (7)$$

Quantification of SCCPs, MCCPs, or LCCPs in each sample was then performed by first applying Eqs. 2, 3, and 5 to obtain the overall %Cl of CPs in the sample, then using the appropriate version of Eq. 7 to calculate the Sample RF. Finally, the concentration of SCCPs, MCCPs, or LCCPs in the sample was calculated from the Sample RF using Eq. 8.

$$Concentration\ of\ CPs\ (Sample) = \frac{\sum Normalized\ Congener\ Peak\ Areas\ (Sample)}{RF\ (Sample)} \quad (8)$$

Table S1. Information of 96 Canadian Consumer Products.

Category	Product ID#	Description	New/Used
Clothing and Bags	6	White Cotton T-Shirt	Used
	9	Blue Denim Jeans (women's)	Used
	19	Yellow Cotton T-Shirt	Used
	20	Blue Cotton Shirt	Used
	28	Navy Blue Cotton Shirt	Used
	29	Pink and White Shirt	Used
	30	Gray Sweater	Used
	31	Blue Denim Jeans	Used
	32	Blue Denim Jeans	Used
	53	Red Cotton T-Shirt	Used
	54	Yellow Cotton T-Shirt	Used
	63	Dark Gray Socks	Used
	60	Synthetic Leather High-Heeled Boot (Tongue)	Used
	59	Synthetic Leather High-Heeled Boot (Tread)	Used
	88	White Running Shoe (Tread)	Used
	89	White Running Shoe (Interior Heel Cushioning)	Used
	61	Beige Canvas Reusable Shopping Bag	Used
	62	Black Rope Handle (from Reusable Shopping Bag)	Used
	64	Black Backpack Strap	Used
Indoor Furnishings	10	White Plush Carpet	Used
	33	Gray Carpet	Used
	47	Black Carpet	Used
	65	Dark Gray Cat Tree Carpeting	Used
	2	White Indoor Paint (Living Room)	Used
	48	White Indoor Paint (Living Room)	Used
	52	White Indoor Paint (Bathroom)	Used
	66	White Indoor Paint (Bathroom)	Used
	18	White Shower Curtain	Used
	67	White Curtain Slats	Used
	46	Vinyl Heating Bag	Used
	1	Yellow Patterned Bed Sheet	Used
	36	Pale Blue Pillow Case	Used
Toys	34	Black Stuffed Animal (Fur)	Used

	35	Pink Stuffed Animal (Fur)	Used
	39	Yellow Plastic Rattle Handle	Used
	93	Orange Plastic Miniature Pony	New
	94	Blue Stretchy Worm Toy	New
	95	Yellow Bouncy Ball	New
	96	Orange-Yellow Bouncy Ball	New
	38	Green Rubber Toddler's Chew Toy (Glove)	Used
	58	Turquoise Foam Dolphin	Used
	91	Red Foam Ball	New
	92	Brown Foam Fake Poop	New
	85	Hard Foam Water-Absorbent Toy Alligator	New
	37	Vinyl Stickers (Finding Dory)	New
	68	Vinyl Stickers (Princesses)	Used
	27	Blue Toy Racecar	Used
	40	Green Building Toy	Used
	49	White Building Toy	Used
	80	Green Children's Cookie Cutters	New
	81	Black Miniature Hockey Stick	New
	82	Pink Miniature Toy Saxophone	New
	83	Green "Grabber" Toy	New
	84	Orange Toy Giraffe	New
	86	Purple Toy Comb	New
	87	Black Toy Racecar	New
Electronics	7	Headphone Wires (Plastic Sheath)	Used
	21	Computer Wires (Plastic Sheath)	Used
	8	Over-Ear Headphones	Used
Paper and Packaging	72	Orange Paper Envelope	New
	69	Green-Printed Cardboard Box	New
	70	Unmarked Cardboard Box	Used
	71	White Cardstock Greeting Card	Used
	73	Black/Purple Cardboard Toy Packaging	New
	74	Green Cardboard Toy Packaging	New
	75	Blue/Yellow Cardboard Toy Packaging	New
	76	Purple Cardboard Toy Packaging	New
	77	Red/Yellow Cardboard Toy Packaging	New

	78	Blue Cardboard Toy Packaging	New
Personal Care Products	3	Face Wash	Used
	11	Hydrating Lotion	Used
	12	Facial Cleanser	Used
	17	Hand Cream	Used
	22	Skin Cream	Used
	26	Face Cleanser	Used
	50	Skin Cream	Used
	57	Hand Cream	Used
	15	Body Wash	Used
	25	Body Wash	Used
	4	Shampoo	Used
	14	Shampoo	Used
	16	Hair Conditioner	Used
	23	Shampoo	Used
	43	Hair Gel	Used
	44	Shampoo	Used
	51	Shampoo	Used
	55	Shampoo	Used
	56	Conditioner	Used
	13	Toothpaste	Used
	24	Toothpaste	Used
	5	Hand Soap	Used
	41	Hand Soap	Used
Cleaning Products	42	Bathroom Cleaner	Used
	45	Dish Soap	Used
Other	90	Metallic-Coloured Twist Ties	Used
	79	Black Scissors Handle	Used

66 **Table S2.** Instrumental detection limits (IDL, μg/L) and method detection limits (MDL, ng/g)

67 for CPs.

CP	IDL by Direct API[2] (μg/L)	IDL by LC-DCM[2] (μg/L)	IDL (μg/L)	MDL (ng/g)
SCCPs	600-900	70-200	0.52	2.97
MCCPs	200-300	20-100	0.41	10.2
LCCPs	100-200	10-60	0.48	2.31

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Table S3. Recoveries (n=3) of CP mixtures across three representative samples.

CP	Hand Cream (n=3)	Toy (n=3)	Electronic Wire (n=3)
SCCPs	91.1 ± 7.6	87.2 ± 6.4	74.0 ± 9.4
MCCPs	86.5 ± 7.1	86.3 ± 8.6	67.0 ± 7.1
LCCPs	92.5 ± 10.6	95.4 ± 9.0	52.4 ± 9.3

Table S4. Manufacturer-provided and experimentally determined chlorine contents for the 6 technical CP mixtures used.

Technical Mixture Groups	Manufacturer	Experimentally Determined Chlorine
SCCPs ($C_{10}-C_{13}$)	51.5%	55.8%
SCCPs ($C_{10}-C_{13}$)	63%	63.0%
MCCPs ($C_{14}-C_{17}$)	42%	49.8%
MCCPs ($C_{14}-C_{17}$)	57%	57.5%
LCCPs ($C_{18}-C_{20}$)	36%	43.6%
LCCPs ($C_{18}-C_{20}$)	49%	49.9%

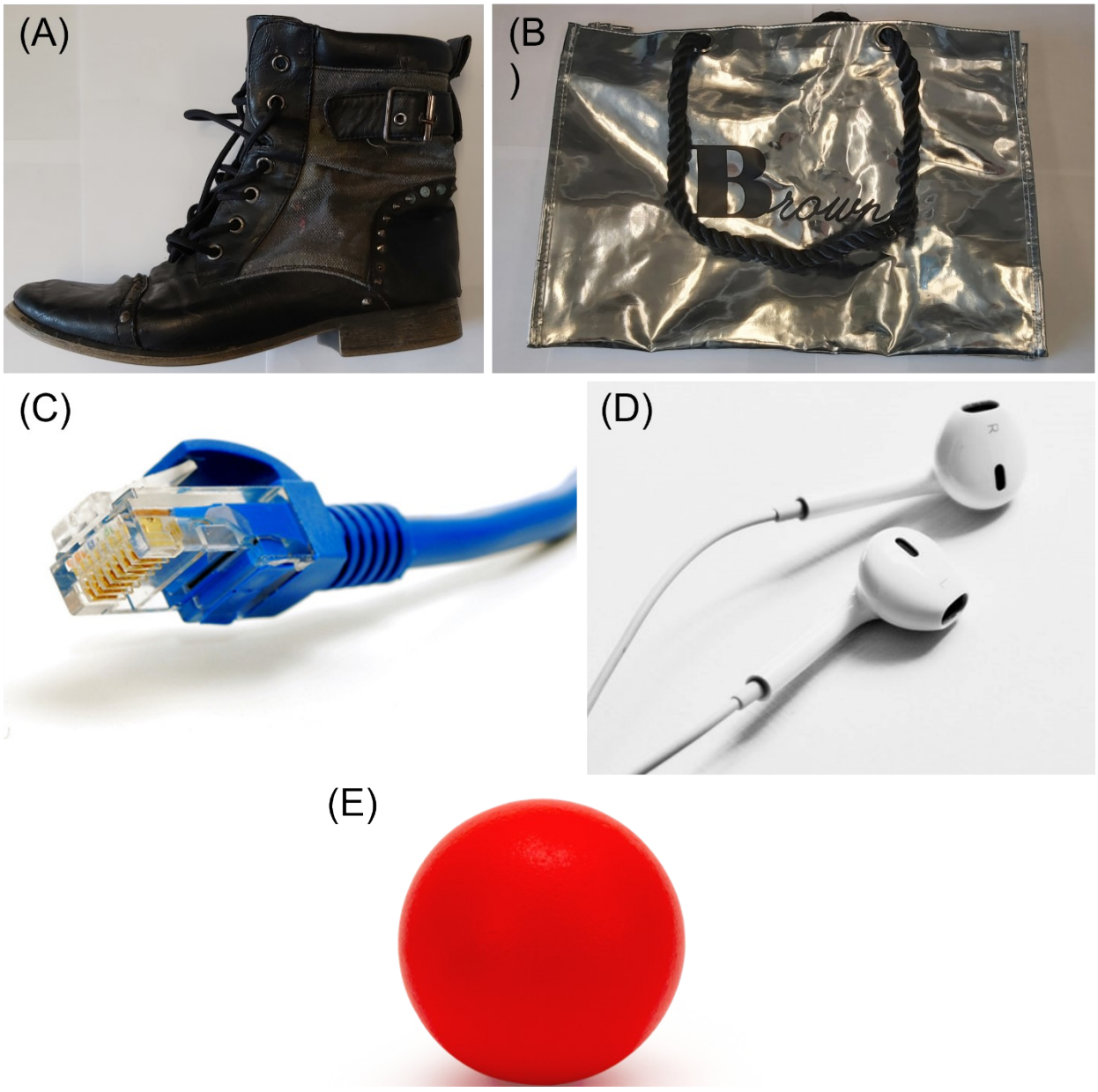

Figure S1. Photos of indoor products with high concentrations of CPs. Photos A and B are of real sampled products, while photos C through E are representative of the original products. (A) A synthetic leather women's boot (Product #60, 0.55 mg SCCPs/g, 0.21 mg MCCPs/g and 0.08 mg LCCPs/g). (B) A canvas reusable shopping bag (Product #61, 4.8 mg SCCPs/g, 2.6 mg MCCPs/g and 1.2 mg LCCPs/g). (C) Ethernet cable covering (Product #21, 9.34 mg SCCPs/g, 18.7 mg MCCPs/g and 5.79 mg LCCPs/g). (D) Plastic wire sheath from headphones (Product #7, 3.01 mg SCCPs/g, 5.05 mg MCCPs/g and 0.63 mg LCCPs/g). (E) Red foam ball toy (Product #91, 2.02 mg SCCPs/g, 3.41 mg MCCPs/g and 0.14 mg LCCPs/g)

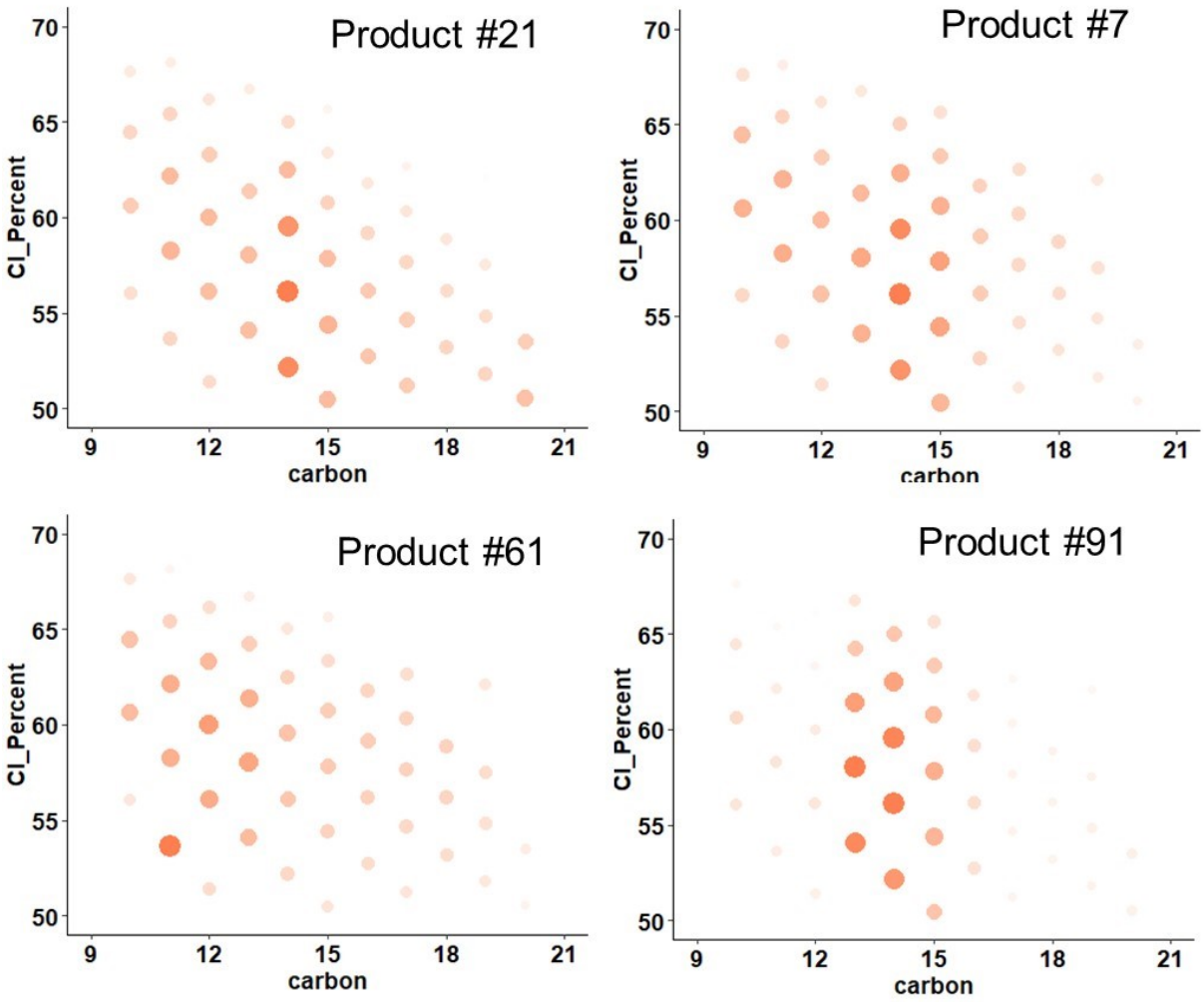

Figure S2. Different profiles of Homologues of chlorinated paraffins in four representative products. Cl_Percent indicates the percentage of chlorine in corresponding chlorinated paraffin Homologues. Size and color of the dot is proportional to abundances.

References

1. Reth, M.; Zencak, Z.; Oehme, M. New quantification procedure for the analysis of chlorinated paraffins using electron capture negative ionization mass spectrometry. *J. Chromatogr. A* **2005**, *1081*, 225–231.

2. Li, T.; Wan, Y.; Gao, S. X.; Wang, B. L.; Hu, J. Y. High-throughput determination and characterization of short-, medium-, and long-chain chlorinated paraffins in human blood. *Environ. Sci. Technol.* 2017, *51*, 3346-3354.