Supporting Information

Complex Mixtures of Chlorinated Paraffins Found in Hand Wipes of a Norwegian Cohort

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Sample collection and storage

The participants were advised to keep their hands unwashed for at least 60 min before collecting the hand wipes. Two sterile gauze pads (3×3 in., Swift First Aid Inc. Valencia, CA, USA) were immersed in 3 mL isopropanol and then used to wipe the palm and the back of both hands, respectively, from wrist to fingertips. Left and right hands were sampled separately but extracted and analyzed together, providing one measurement per participant. Both pieces of gauze pad were stored in a 60 mL amber glass jar at −20 °C until analysis. Field blank samples were taken by soaking a gauze pad in isopropanol and placing it directly into a glass jar. After sample collection, the participants were asked to complete a questionnaire regarding indoor environment characteristics, type and number of consumer products, as well as some personal behaviors. Within a 2-day collection period, the participants collected 4 sets of hand wipes, during the first visit in Day 1, in the evening of Day 1, in the morning of Day 2 and before lunch in Day 2. The sample analyzed in the current study was the last collected sample. A total of 60 hand wipe samples and 15 field blanks (two field blanks were lost in the analytical process) were collected from 60 participants for CP analysis.

Instrumental analysis

APCI-Orbitrap-HRMS (Q Exactive, Thermo Fisher Scientific, San Jose, USA) was operated in full-scan mode (m/z 250 – 2000) with a resolution of 120 000 FWHM. The instrumental settings were optimized using a SCCP mixture (51.5% Cl, 15 ng/μL) and a LCCP mixture (Witaclor 549, 49% Cl, 5 ng/μL) as follows: injection volume 3 μL, mobile phase flow rate 0.100 mL/min, DCM flow rate 0.010 mL/min, capillary temperature 250 °C, Aux (auxiliary) gas heater temperature 250 °C, spray current 5.7 μA, maximum IT (ion time) 250 ms, AGC (automatic gain control) target 5e6, sheath gas flow rate 17 arbs, and Aux gas flow rate 1 arb.

Uncertainty analysis of profile deconvolution used for CP quantification

Quantification of CPs yield only a total concentration of the mixture as a single value. The criterion is that the reference mixture of CPs selected for quantification should have a carbon-chlorine profile as similar as possible with the profile in each sample,[1] otherwise, the deviation can be up to 1000%.[2, 3] Bogdal et al.[4] quantified the similarity between the profiles of reference CPs and sample using the goodness of fit (R^2), with R^2=1 indicating a perfect fit and the least deviation. Both Bogdal et al.[4] and Brandsma et al.[5] defined $R^2 = 0.50$ as a cut-off threshold for quantifying CPs based on an uncertainty test using different CP reference standards with known concentrations. The uncertainty test in our study (Figure S1) showed a mean deviation of 40% in quantification difference when $R^2 = 0.50$. The deviation seems to be within a reasonable range compared with mean deviations of 49-96% of SCCPs with presence of MCCPs in a recent interlaboratory study with participants from 18 countries.[6] Therefore, we continued using the criterion of R^2>0.50 as the threshold of a valid quantification of CPs using profile deconvolution.

Table S1. Descriptive statistics for chemical contaminants measured in the same hand wipe samples.

		Mass (ng/participant)			Reference
		mean	median	min-max	
CPs	vSCCPs	1.3	<0.70	<0.70-13	Present study
	SCCPs	280	160	22-2400	Present study
	MCCPs	840	490	33-7400	Present study
	LCCPs	570	150	10-8500	Present study
	sumCPs	1700	950	43-18000	Present study
PBDEs	sumPBDE	6.3	2.9	0.44-64	Tay et al. (2018)[7]
HBCDDs	sumHBCDD	680	180	49-8900	Tay et al. (2018)[7]
EHFRs	TBBPA	1300	570	<30-11000	Tay et al. (2018)[7]
	sumEHFR	1300	570	31-11000	Tay et al. (2018)[7]
PFAS	6:2 diPAP	3.3	0.54	-87	Poothong et al. (2019)[8]
	8:2 diPAP	4.7	0.41	-213	Poothong et al. (2019)[8]
OPEs	ΣOPEs		192	20-14100	Xu et al. (2016)[9]
phthalate esters	DEHP		5570*		Giovanoulis et al. (2018)[10]
	DiNP		5690*		Giovanoulis et al. (2018)[10]
	DPHP		360*		Giovanoulis et al. (2018)[10]

PFAS: Perfluoroalkyl Substances; EHFRs: Emerging halogenated flame retardants; PAP: Polyfluoroalkyl phosphate ester; OPEs: Organophosphate ester. TBBPA and diPAP were the most abundant EHFRs and PFAs, respectively, found in the hand wipes, which were thus included in the table.

*unit: pg/cm^2

Table S2. Relative contributions of chlorinated paraffin standards in pattern reconstruction of individual hand wipe samples.

Sample	R^2	***Relative contributions from SCCP products***					***Relative contributions from MCCP products***							***Relative contributions from LCCP products***				
		Witaclor 149	***SCCP 51.5% Cl***	***SCCP 55.5% Cl***	***SCCP 63% Cl***	***Hüls 70C***	***MCCP 42% Cl***	***MCCP 52% Cl***	***MCCP 57% Cl***	***Cloparin 49st***	***Cloparin 50***	***Cereclor S52***	***Hüls 52G***	***LCCP 36% Cl***	***LCCP 49% Cl***	***Uniclor 40***	***Hüls 40N***	***Witaclor VP549***
HW01	0.58	1%	9%		5%		37%	1%	20%	15%	1%	4%	0%	2%	0%	1%	2%	0%
HW02	0.83	1%	12%		4%		20%	1%	8%	30%	2%	15%		6%	0%		1%	0%
HW03	0.70	1%	2%	0%	1%		19%			29%				38%	0%	1%	9%	0%
HW04	0.79		0%	0%	0%		0%	74%	25%	0%				0%	0%	0%	0%	0%
HW05	0.83	1%	9%		5%		30%	1%	11%	12%	1%	3%	0%	22%	0%	1%	3%	0%
HW06	0.72	1%	0%		1%		18%	1%	0%	3%	1%	2%	1%	68%	0%	1%	4%	0%
HW07	0.78	1%	3%	8%	3%		46%	1%	7%	18%	1%	0%	0%	11%	0%	0%		0%
HW08	0.85			27%	5%		24%	4%	15%		9%		12%		3%			0%
HW09	0.88	1%	5%	3%	0%	0%	25%	1%	20%	28%	1%	5%	3%	7%	0%	1%	1%	0%
HW10	0.74	1%	4%	0%	2%		58%	1%	5%	13%	1%	2%	0%	11%	0%	1%	2%	0%
HW11	0.66	1%	5%		5%		6%	1%		57%	1%	2%	0%	16%	0%	1%	2%	0%
HW12	0.85	1%	9%	1%	1%		33%	1%	8%	33%	1%	1%	0%	11%	0%	1%	0%	0%
HW13	0.87	1%	10%	3%	2%		24%	1%	13%	28%	1%	3%	0%	12%	0%	1%	1%	0%
HW14	0.65	0%	5%	0%	0%		28%		18%	37%	1%		0%	9%	0%	1%	1%	0%
HW15	0.81	1%	4%	6%	1%		5%		11%	58%	1%			8%	2%	0%	2%	0%
HW16	0.84	0%	4%	2%	1%		18%		5%	20%		20%	24%	6%		0%	1%	0%
HW17	0.80	1%	9%	4%	4%		31%	1%	20%	16%	1%	4%	0%	6%	0%	1%	2%	0%
HW18	0.75	0%	4%	0%	2%		36%	1%	2%	13%	1%	2%	27%	10%	0%	1%	1%	0%
HW19	0.88	1%	1%	4%	0%	0%	23%	1%	15%	20%	1%	4%	14%	14%	0%	1%	1%	0%
HW20	0.61	1%	4%	4%	2%		24%	1%	47%	7%	1%	6%			0%	1%	1%	0%
HW21	0.56	1%	10%		5%		34%	1%	20%	16%	1%	4%	0%	3%	0%	1%	3%	0%
HW22	0.89		13%	3%	3%		19%	7%	11%	23%	4%	3%	0%	10%	3%		1%	1%
HW23	0.74	1%	10%	0%	2%		36%	1%	15%	22%	1%	4%	0%	5%	0%	1%	1%	0%
HW24	0.64	1%	9%		5%		36%	1%	23%	15%	1%	5%			0%	1%	3%	0%
HW25	0.90			31%	2%		13%	6%	16%		7%	8%	11%	1%	3%			1%
HW26	0.68	1%			0%	0%	41%	1%	11%	23%	1%	4%	14%	0%	0%	1%	2%	0%
HW27	0.80	0%	1%	2%	1%		75%			18%			0%	3%	0%			0%
HW28	0.62	1%	9%	0%	2%		40%	1%	15%	20%	1%	4%	0%	5%	0%	1%	1%	0%

HW29	0.80		12%		2%		28%	0%	15%	28%				14%	0%		0%	0%
HW30	0.82	1%	9%		5%		15%	1%	15%	14%	1%	4%	0%	29%	0%	1%	4%	0%
HW31	0.74	1%	5%	8%	9%	1%	26%		13%	27%	1%		1%	5%	1%	4%		0%
HW32	0.82		9%	5%	7%		17%	7%	16%	2%	7%	15%		7%	5%			1%
HW33	0.54	1%	7%		5%		35%	1%	22%	15%	1%	4%	0%	5%	0%	1%	2%	0%
HW34	0.71	1%	7%	0%	0%		14%	2%	9%	20%	2%	9%		31%	1%	1%	3%	0%
HW35	0.79	1%	11%		4%		27%	1%	19%	18%	1%	5%	0%	9%	0%	1%	3%	0%
HW36	0.70	1%	9%		4%		18%	1%	17%	34%	1%	6%	0%	6%	0%	1%	2%	0%
HW37	0.85		16%		1%		14%	1%	8%	38%	4%			6%	8%	2%	1%	0%
HW38	0.92		5%	15%	7%		19%	27%	18%		4%			1%	4%		0%	1%
HW39	0.71	1%	9%	3%	6%		29%	1%	21%	15%	1%	4%		5%	0%	1%	2%	0%
HW40	0.81	1%	6%	2%	4%		9%	1%	18%	28%	1%	3%	0%	25%	0%	0%	1%	0%
HW41	0.72	1%	8%	4%	6%		26%	2%	26%	15%	1%	6%	0%	2%	0%	1%	1%	0%
HW42	0.51	3%	1%	1%	0%		31%	3%	9%	14%	3%	2%	0%	22%	1%	2%	5%	0%
HW43	0.66	8%	3%	5%	2%		24%	6%	3%	38%	1%	4%		2%	3%		0%	
HW44	0.72	2%	1%	0%		0%	46%	3%		11%	2%	26%		5%	1%	1%	0%	0%
HW45	0.88		8%	4%	2%		19%	5%	16%	29%		3%		5%	1%	2%	5%	
HW46	0.60	1%	8%		5%		38%	1%	13%	13%	1%	4%	0%	11%	0%	1%	2%	0%
HW47	0.59	1%	16%		4%		17%	1%	27%	16%	1%	5%	6%		0%	1%	2%	0%
HW48	0.68	1%	10%		4%		35%	1%	18%	19%	1%	4%	0%	3%	0%	1%	2%	0%
HW49	0.73	1%	6%	13%	4%		24%	1%	11%	9%	1%	3%	14%	10%	0%	1%	2%	0%
HW50	0.77	0%	1%	0%	1%		35%			27%				35%	0%	0%	0%	0%
HW51	0.60	1%		0%	0%	1%	19%	2%	10%	54%	2%	9%	0%		0%	1%	1%	0%
HW52	0.81	1%	10%	3%	3%		13%	1%	17%	38%	2%	6%		2%	0%	1%	2%	0%
HW53	0.69	1%	12%	0%	3%		38%	2%	12%	16%	1%	9%		4%	0%	2%	0%	0%
HW54	0.88	1%	7%	2%	2%		15%	2%	12%	34%	2%	13%		8%	1%	2%	0%	0%
HW55	0.78	1%	7%	0%	4%		35%	1%	9%	14%	1%	3%	14%	8%	0%	1%	2%	0%
HW56	0.69	1%	10%		6%		30%	1%	21%	14%	1%	4%	0%	7%	0%	1%	3%	0%
HW57	0.53	1%	4%	2%		1%	42%	1%	23%	15%	1%	7%			0%	1%	1%	0%
HW58	0.78	0%	5%		3%	0%	32%	1%	13%	11%	1%	3%	25%	6%	0%	1%	1%	0%
HW59	0.69	5%	2%	2%	0%	0%	0%	5%	18%		5%	18%			1%	15%	27%	1%
HW60	0.72	1%	7%	0%	3%	0%	20%	2%	18%	30%	1%	10%		4%	0%	2%	1%	0%

Table S3. Goodness of fit (R^2) between congener group profile of vSCCPs in CP-52 and that profile in individual hand wipe samples.

Sample	**R^2**	**Sample**	**R^2**	**Sample**	**R^2**
HW01	0.97	HW21	–	HW41	0.80
HW02	– [a]	HW22	0.96	HW42	–
HW03	0.44[b]	HW23	–	HW43	0.84
HW04	0.75	HW24	0.74	HW44	–
HW05	–	HW25	0.43[b]	HW45	0.69
HW06	–	HW26	–	HW46	–
HW07	–	HW27	0.69	HW47	–
HW08	–	HW28	–	HW48	–
HW09	0.89	HW29	0.83	HW49	0.73
HW10	–	HW30	–	HW50	–
HW11	0.42[b]	HW31	–	HW51	–
HW12	–	HW32	–	HW52	–
HW13	–	HW33	–	HW53	–
HW14	–	HW34	–	HW54	–
HW15	0.86	HW35	–	HW55	0.61
HW16	0.67	HW36	–	HW56	0.76
HW17	–	HW37	–	HW57	–
HW18	0.96	HW38	–	HW58	0.43[b]
HW19	0.43[b]	HW39	–	HW59	0.52
HW20	0.78	HW40	–	HW60	–

a. <LOD; b. $R^2<0.50$.

Table S4. Recoveries determined from spiking experiments.

CP mixture	spiked level (ng)	% recovery in each of the spiking experiments before IS correction†							% recovery after IS correction
		1st	2nd	3rd	4th	5th	6th	mean	mean
SCCPs (51.5%Cl + 63.0%Cl)	300 ng + 300 ng	75	82	82	–	–	–	79	103
MCCPs (42.0%Cl + 57.0%Cl)	300 ng + 300 ng	61	82	79	–	–	–	74	96
LCCPs (49.0%Cl)	300 ng	103	71	48	–	–	–	74	96
vSCCPs (CP-52)	9.4 ng*	–	–	–	84	70	65	73	100
^{13}C-CP internal standard (IS)	10 ng	77	85	70	77	68	74	75	–

*1000 ng CP-52 was spiked, 0.94% of which was vSCCPs[11].

† IS-corrected recovery = recovery of vS/S/M/LCCPs ÷ recovery of ^{13}C-CP internal standard (IS), which was calculated in each of the spiking experiments, respectively.

Table S5. Gender-specific constants used for the estimation of hand surface area

	a	b	c
male	0.0257	0.573	-0.128
female	0.0131	0.412	0.0274

(Source: U.S. EPA Exposure Factors Handbook[12])

Table S6: Absorption fractions used for exposure assessment

	molecular weight	**Log K_{OW}**	**Absorption fraction**	**Estimated absorption fraction**
vSCCPs	335 ($C_9H_{14}Cl_6$)	5.99[13]		0.27
SCCPs	363 ($C_{11}H_{18}Cl_6$)	4.10-8.67[14]		0.27
MCCPs	405 ($C_{14}H_{24}Cl_6$) 516 ($C_{17}H_{28}Cl_8$)	5.56-8.38[14]		0.34
LCCPs	461 ($C_{18}H_{32}Cl_6$) 545 ($C_{24}H_{44}Cl_6$) 713 ($C_{36}H_{68}Cl_6$)	6.58-11.34[14]		0.13
TBP-AE	370.8	5.80		0.27
BDE-28	406.9	5.94[15]	0.27[16]	
BDE-47	485.8	6.81[15]	0.33[16]	
TBBPA	543.9	5.90	0.30[b]	
BDE-99	564.7	7.32[15]	0.34[16]	
***α*-HBCDD**	641.7	6.78[17]	0.36[b]	
***β*-HBCDD**	641.7	6.78[17]	0.31[b]	
***γ*-HBCDD**	641.7	6.78[17]	0.27[b]	
BDE-153	643.6	7.90[15]	0.37[16]	
***anti*-DDC-CO**	653.7	11.11[17]	0.09[a]	
***syn*-DDC-CO**	653.7	11.11[17]	0.09[a]	
BTBPE	687.6	9.41[17]	0.11[a]	
BEH-TEBP	706.1	11.04[17]	0.10[a]	
BDE-183	722.5	8.27[15]	0.13[16]	
BDE-209	959.2	9.97	0.08[16]	
DBDPE	971.2	11.96[17]	0.11[a]	

[a]: Frederiksen et al. 2016,[17] values were obtained by summing mean distribution of FRs in epidermis and dermis compartments

[b]: Abdallah et al. 2015,[16] values were obtained by summing distribution of FRs in directly absorbed fraction and skin-epidermis (depot)

Table S7. Characteristic of the study group/indoor environment questionnaire parameters and the median amounts of CPs (with detection frequencies above 80%) in the hand wipes (ng).

	n	**Median (Interquartile Range: IQR)**			
		SCCPs	**MCCPs**	**LCCPs**	**sumCPs**
Gender of participants					
Female	45	180 (97-330)	550 (270-1000)	140 (64-300)	1000 (480-1800)
Male	15	110 (63-230)	390 (170-890)	200 (53-400)	640 (360-1500)
% median difference [a]		46	34	38	47
Age of participants					
<41 years old	30	110 (63-300)	470 (180-960)	89 (42-300)	800 (320-1800)
≥41 years old	30	180 (110-260)	520 (340-1100)	210 (85-380)	1200 (550-1900)
% median difference [a]		46	10	79	37
Owning a sofa					
Yes	45	180 (98-330)	630 (300-1200)	170 (76-420)	1300 (510-2200)
No	15	63 (45-230)	220 (110-500)	84 (32-280)	330 (190-1200)
% median difference [a]		97*	95*	65	120*
Work mainly in					
Office	40	160 (98-270)	480 (280-910)	160 (64-320)	970 (500-1500)
Lab	20	210 (62-460)	720 (180-1500)	140 (44-410)	1400 (310-2600)
% median difference [a]		28	39	16	33
Percent work time with electrical/electronic equipment					
<80%	22	190 (73-320)	510 (290-1000)	180 (55-400)	1100 (460-1800)
80%-100%	38	150 (93-280)	480 (260-1000)	140 (66-340)	970 (460-1700)
% median difference [a]		25	4	21	11
Work hours					
≤ 8 hours	45	170 (68-280)	500 (260-950)	160 (52-410)	970 (450-1500)
> 8 hours	15	180 (110-510)	460 (280-1400)	140 (83-290)	1000 (500-2300)
% median difference [a]		8	7	15	6
Residence house/apartment built (data available for 55 participants)					
≤ 11 years, after the 2002 ban	8	110 (56-230)	400 (260-680)	84 (68-250)	710 (390-1100)
> 11 years	47	180 (90-290)	500 (260-1100)	150 (58-360)	1000 (460-2000)
% median difference [a]		52*	22	57	37
Size of the home area					
≤ 80 m^2	23	160 (94-310)	470 (250-960)	94 (51-250)	930 (370-1500)
80-120 m^2	18	190 (73-390)	520 (270-1200)	190 (54-360)	1100 (480-2100)
>120 m^2	19	160 (92-200)	440 (270-1000)	220 (87-440)	1000 (460-1700)
Statistical significance [b]		p>0.05	p>0.05	p>0.05	p>0.05
How long people had lived in the home					
≤ 2 years	21	160 (97-370)	470 (290-1000)	140 (83-120)	970 (480-1800)
2-6 years	20	110 (64-210)	460 (160-960)	76 (29-270)	680 (300-1400)
>6 years	19	200 (130-370)	850 (250-1500)	220 (120-430)	1400 (510-2400)
Statistical significance [b]		p>0.05	p>0.05	p>0.05	p>0.05
No. of children in the home					
0	30	140 (71-260)	420 (240-850)	86 (47-200)	690 (350-1400)
1	11	270 (140-430)	880 (450-1300)	240 (180-1600)	1600 (940-3600)
>1	19	160 (79-270)	520 (240-1200)	200 (56-440)	1100 (450-2000)
Statistical significance [b]		p>0.05	p>0.05	p>0.05	p<0.05
No. of TVs					
0	10	180 (97-260)	630 (370-1100)	160 (47-380)	1300 (610-2000)
1	35	120 (64-220)	280 (190-850)	110 (50-200)	510 (330-1300)
>1	15	190 (140-280)	720 (360-1400)	320 (150-450)	1200 (760-2300)
Statistical significance [b]		p>0.05	p>0.05	p>0.05 [d]	p>0.05

	n	Median (Interquartile Range: IQR)			
		SCCPs	**MCCPs**	**LCCPs**	**sumCPs**
No. of (mobile) phones					
<2	12	110 (62-280)	540 (170-1100)	93 (42-250)	780 (290-1700)
2	23	180 (97-270)	470 (290-880)	190 (83-340)	660 (320-1700)
>2	25	180 (89-310)	490 (220-1400)	150 (64-340)	1100 (510-1800)
Statistical significance [b]		p>0.05	p>0.05	p>0.05	p>0.05
No. of laptops/tablets/PCs					
<3	23	190 (95-310)	630 (370-1100)	160 (47-380)	1300 (610-2000)
3-4	22	120 (64-220)	280 (190-850)	110 (50-200)	510 (330-1300)
>4	15	190 (130-280)	720 (360-1400)	320 (150-470)	1200 (760-2300)
Statistical significance [b]		p>0.05	p>0.05	p>0.05	p>0.05
Floor material					
Parquet	42	170 (71- 280)	490 (270-1000)	150 (55-420)	950 (480-1800)
Wood	8	210 (110-310)	680 (260-1200)	120 (58-260)	970 (410-1600)
Laminate	5	290 (230-490)	960 (950-1800)	160 (95-220)	1400 (1400-2400)
Flooring [c]	3	110 (100-130)	340 (260-360)	190 (120-400)	640 (480-900)
Wall-to-wall carpet	1	190	720	340	1200
Other	1	18	51	63	130
Statistical significance [b]		p>0.05	p>0.05	p>0.05	p>0.05

* p<0.05, Mann−Whitney test;
[a] median difference in concentration of two categories in %, $((A - B)/((A + B)/2)) \times 100$;
[b] Kruskal-Wallis test;
[c] floor material which comprises e.g. PVC and linoleum;
[d] $p < 0.05$ and r = 0.15 using Spearman rank correlation coefficients.

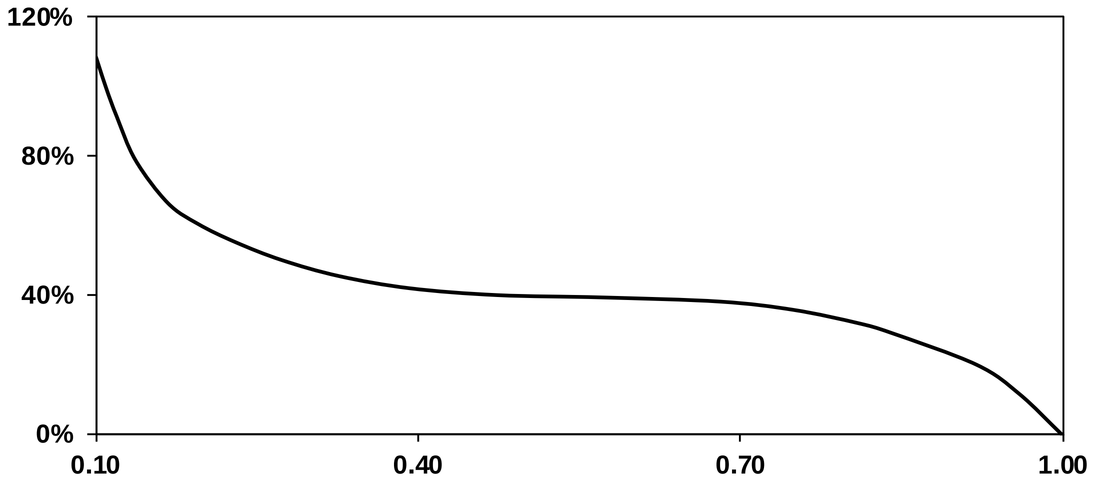

Figure S1. Evolution of the mean deviation (%) of calculated concentration from the assigned concentration as a function of the goodness of fit (R^2) for a simulation of a mixture of SCCPs 55.5%Cl, MCCPs 52.0%Cl, and LCCPs 49.0%Cl.

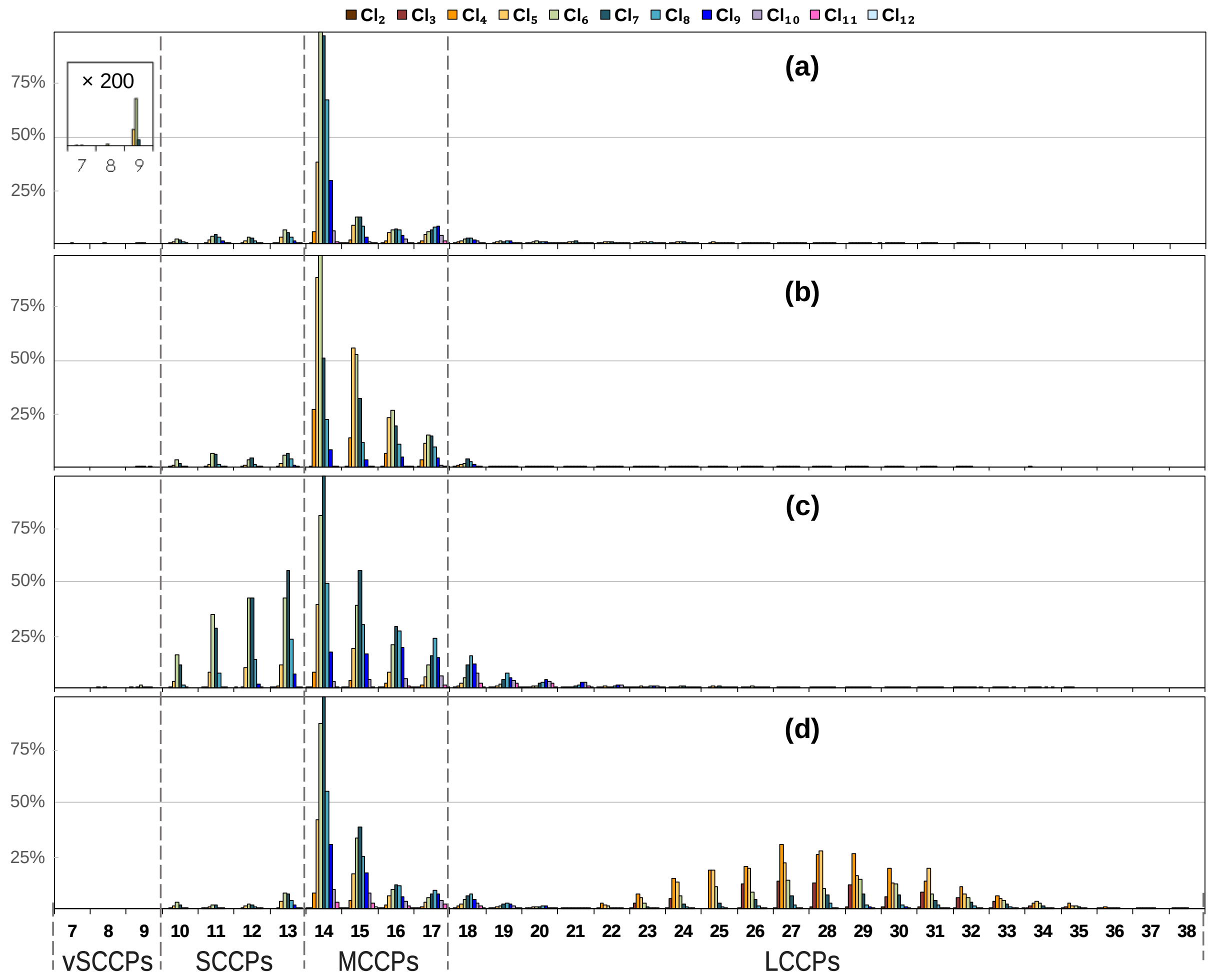

Figure S2. Congener group profiles of chlorinated paraffins in selected hand wipes from the Norwegian cohort. The vertical axis represent percent relative abundance; all of the horizontal axis represent carbon chain length.

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