Supporting Information - Partitioning of chlorinated paraffins (CPs) to *Daphnia magna* overlaps between restricted and in-use categories

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Determination of the organic carbon content in *D. magna*

"Organic carbon was determined by combustion on a Carlo Erba NC2500 analyser connected via a split interface to reduce the gas volume to a Finnigan MAT Delta V mass spectrometer. The percentage of organic carbon was determined using appropriate standards, with a known % of organic carbon (Acetanilide, 71.09% C). The relative error was <1%.

Figure S1. Complete congener profile of Cereclor S45 (C_{13}-C_{18}, 45% Cl)..

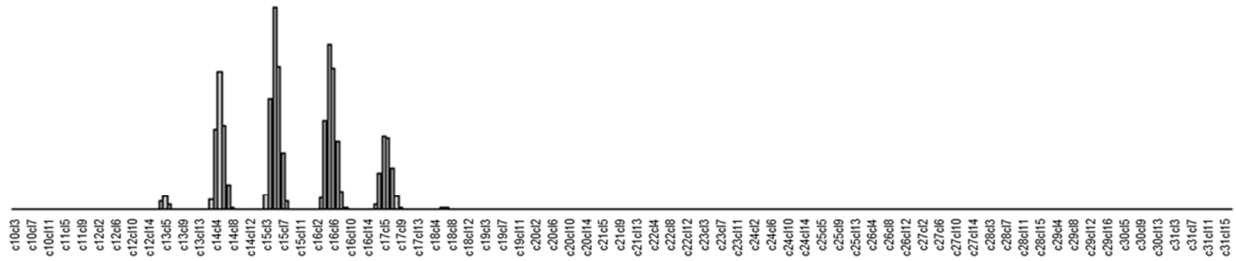

Figure S2. Complete congener profile of Cereclor 50LV (C_9-C_{14}, 50% Cl).

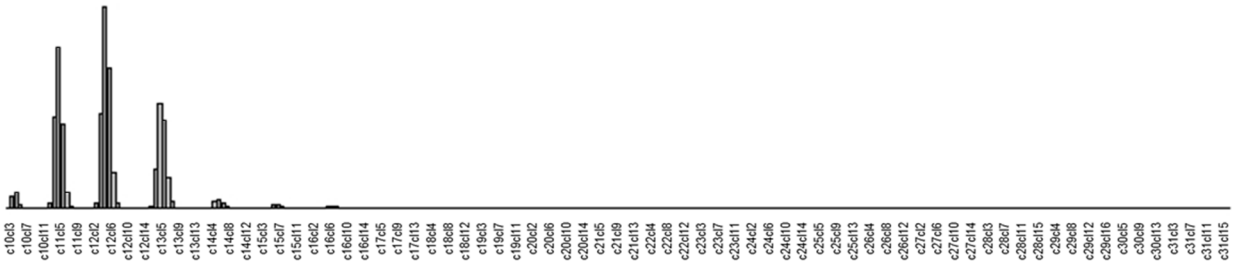

Figure S3. Complete congener profile of Huels 70C (C_9-C_{14}, 70% Cl).

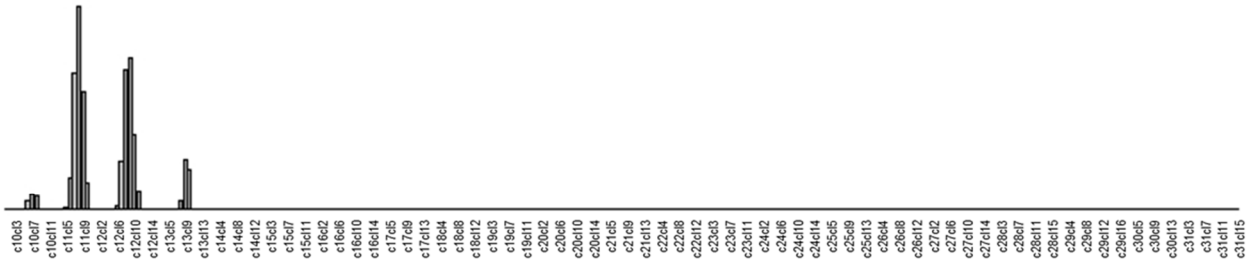

Figure S4. Complete congener profile of Cereclor 42 (C_{10}-C_{14}, C_{21}-C_{31}, 42% Cl).

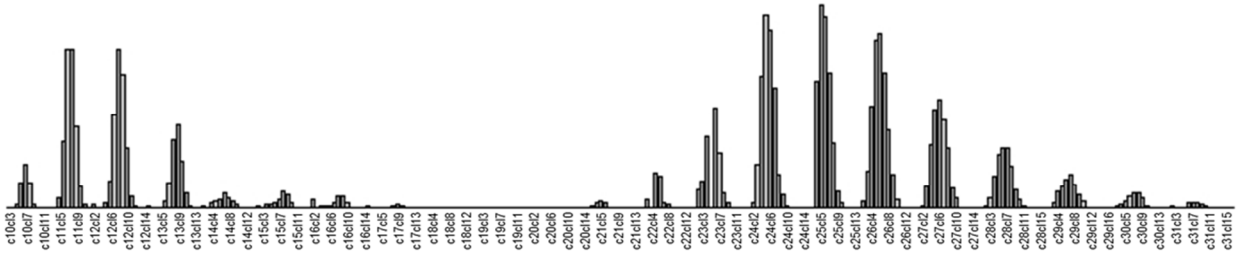

Figure S5. Complete congener profile of CP-52 (C_9-C_{30}, 52% Cl).

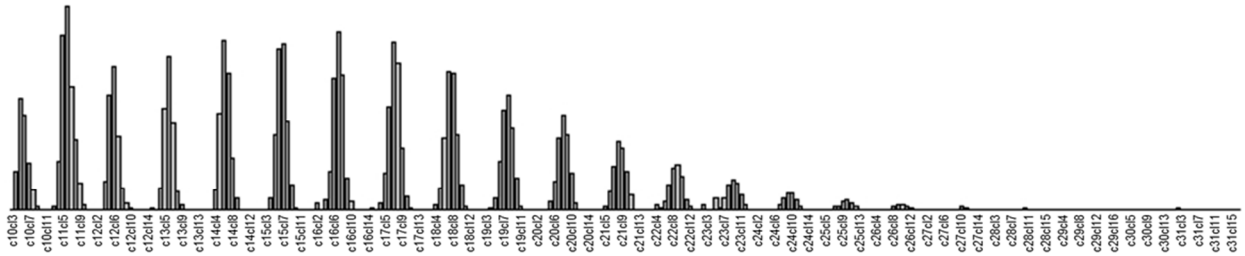

Table S1. Calculated post quantification mass balance in the passive dosing vial (mg CPs) for the low (5 mg CPs.g-1 silicone) and high (5 mg CPs.g-1 silicone) concentration and their loading efficiency (%=calculated mass balance/initially added amount of CPs). n=9 per CP technical mixture per concentration.

Commercial name	Mass balance / % mg CPs in water		Loading efficiency / %	
	Low concentration	High concentration	Low concentration	High concentration
Cereclor S45	0.32±0.49	0.41±0.42	57.5	53.8
Cereclor 50LV	0.06±0.04	0.05±0.04	34.7	38.7
Huels 70C	0.004±0.001	0.004±0.001	58.8	38.6
Cereclor 42	0.05±0.0.04	0.21±0.09	28.1	15.5
CP-52	0.002±0.001	0.002±0.001	27.7	15.1

Table S2. Summary of the results obtained in the silicone method loading experiments, method 1 being the removal of the CP/isooctane solution from the passive dosing vial after 72 hours and method 2 being the evaporation of the CP/isooctane solution with a gentle stream of nitrogen after 72 hours of contact with the silicone.

Method	CPs in silicone (mg/g silicone)	
	Cereclor 50LV	Huels 70C
1	7.83±0.37	10.33±0.36
2	13.44±1.71	13.22±0.55

Table S3. Average recoveries obtained for water, silicone and daphnia samples for the different CP mixtures.

	Cereclor S45	Cereclor 50LV	Huels 70C	Cereclor 42	CP-52	Overall
Water samples	86±18.4	116±37.5	90±30	141±40.6	83±17.5	103%
Silicone samples	127±29.0	142±78.0	165±19.4	145±11.4	143±18	145%
Daphnia samples	117±16	117±16	-	-	117±16	117%

Table S4. Effect of time on the log $K_{silicone\text{-}water}$. A linear model was applied to evaluate the presence of significant differences between observations over time (24-168 hours) F-statistic indicates how big is the difference from time points, and the p-value is calculated from the F-statistic in this model. No statistically different observations are identified (p>0.05) and therefore no influence of time is assumed.

	Concentration	F-statistic	df	p-value
Cereclor S45	Low	0.068	6	0.93
	High	2.6	4	0.19
Cereclor 50LV	Low	0.40	6	0.69
	High	0.28	6	0.77
Huels 70C	Low	0.22	6	0.81
	High	0.16	6	0.86
Cereclor 42	Low	0.44	6	0.66
	High	1.6	6	0.26
CP-52	Low	1.60	6	0.28
	High	0.52	6	0.62

Table S5. Two sample t-test for the effect of concentration (high and low) in log $K_{silicone\text{-}water}$. p-value shows if the observations corresponding to the two concentrations are statistically different ($p<0.05$).

	t-value	df	p-value
Cereclor S45	-0.12	14	0.90
Cereclor 50LV	-1.5	16	0.145
Huels 70C	-0.22	16	0.83
Cereclor 42	3.1	16	0.0057
CP-52	-1.30	16	0.20

Table S6. Summary of the average (±SD 3 replicates per group) log $K_{silicone\text{-}water}$ for the different CP mixtures for the Low (5 mg CPs.g-1 silicone) and High (10 mg CPs.g-1 silicone) concentrations tested, after 24, 48 and 168 hours of water/silicone contact. Asterisks indicate level of significance: $p \leq 0.05$ (*).

Concentration	Time / h	log $K_{silicone\text{-}water}$				
		Cereclor S45 MCCP	Cereclor 50LV SCCP	Huels 70C SCCP	Cereclor 42 LCCP	CP-52 CP
Low	24	3.85±0.91	3.42±0.18	4.21±0.11	3.19±0.48	5.03±0.27
Low	48	3.90±0.32	3.21±0.37	4.17±0.59	2.94±0.43	4.69±0.09
Low	168	4.07±0.81	3.42±0.39	4.35±0.10	3.21±0.35	4.67±0.41
High	24	4.31±0.44	3.51±0.58	4.34±0.14	2.61±0.10*	4.88±0.22
High	48	3.67±0.42	3.95±0.26	4.21±0.16	2.83±0.31*	4.87±0.34
High	168	3.24[1]	3.46±0.60	4.31±0.29	2.62±0.09*	4.83± 0.20
Averaged		4.10 ± 0.69	3.61 ± 0.78	4.24 ± 0.28	2.64±0.30	4.24 ± 0.52

[1]Only one sample

*Statistically different log $K_{silicone\text{-}water}$ between Low and High concentration for Cereclor 42

Table S7. Results from the generalized linear model testing effects of chlorine content and carbon chain length on log $K_{silicone\text{-}water}$, using short chain as reference for comparison. Asterisks indicate level of significance: $p \leq 0.05$ (*); $p \leq 0.01$ (**); $p \leq 0.001$ (***).

	Estimate	SE	t-value	p-value
Carbon chain length	0.17	0.06	2.7	0.0101
Chlorine content / %	0.008	0.0027	3.0	0.0041

Table S8. Generalized linear models testing effects of the different CP mixtures on log $K_{silicone-water}$, using Cereclor 50LV and Huels 70C (SCCPs) as reference for comparison. Asterisks indicate level of significance: $p \leq 0.05$ (*); $p \leq 0.01$ (**); $p \leq 0.001$ (***).

	Estimate	SE	t-value	p-value
Cereclor 50LV vs				
Cereclor 42	-0.31	0.070	-4.43	***
Cereclor S45	0.13	0.051	2.54	*
CP-52	0.16	0.049	3.30	**
Huels 70C	0.16	0.050	3.280	**
Huels 70C vs				
Cereclor 42	-0.47	0.068	-6.88	***
Cereclor S45	-0.032	0.049	-0.65	0.52
Cereclor 50LV	-0.16	0.049	-3.28	**
CP-52	0.0011	0.047	0.024	0.98

Table S9. Summary of the average (±SD five replicates per group) log $K_{oc\text{-}water}$ for the different CP mixtures at four tested concentrations (0.5, 1, 2, 5 mg CPs g^{-1} silicone) after 48 hours of exposure.

CP mixture	log $K_{oc\text{-}water}$			
	0.5	1	2	5
Cereclor 50LV	6.24±0.811	6.49±0.155	-	-
Cereclor S45	-	4.34±0.334	5.73±0.119	5.59±0.241
CP-52	-	6.85±0.50	5.70±0.42	5.75±0.26
Huels 70C	-	6.76±0.41	-	-

Table S10. Generalized linear models testing the effect of concentration on the log $K_{oc\text{-}water}$ of the different mixtures. P-value indicates statistically different observations between concentrations. Asterisks indicate level of significance: $p \leq 0.05$ (*); $p \leq 0.01$ (**); $p \leq 0.001$ (***).

	Estimate	SE	t-value	p-value
Cereclor 50LV	0.49	0.74	0.67	0.5
Cereclor S45	0.044	0.017	2.6	*
CP-52	-0.036	0.014	-2.5	*

Table S11. Mass balance of CPs in the passive dosing system for the 4 different concentrations tested and their loading efficiency (%=calculated mass balance/initially added amount of CPs). n=5 per CP technical mixture per concentration.

Commercial name	Proportion of CP sorbed to organic carbon (%)				Loading efficiency (%)			
	0.5	1	2	5	0.5	1	2	5
Cereclor 50LV	0.60±0.021	0.39±0.17	-	-	100±5	75±12	-	-
Cereclor S45	-	0.18±0.06	0.10±0.01	0.060±0.009	-	60±24	49±3	43±2
CP-52	-	0.63±0.37	0.11±0.07	0.11±0.07	-	33±14	46±16	32±6

Figure S6. Congener pattern for a water sample for CP mixture Cereclor 42, low concentration, after 24 hours silicone-water contact.

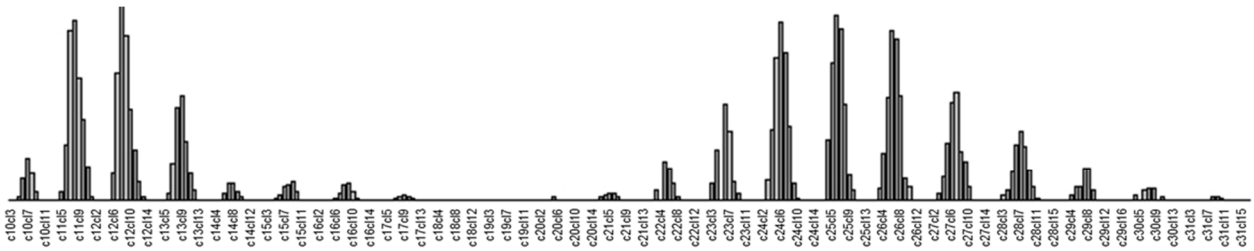

Figure S7. Congener pattern obtained from a *Daphnia magna* sample exposed to CP-52 (5 mg/g silicone).

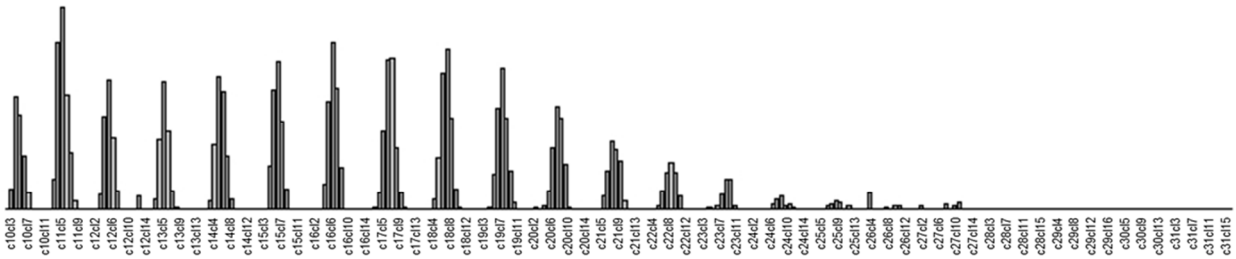

Table S12. General linear models testing effects of the different CP mixtures on the log $K_{oc\text{-}water}$ using Cereclor 50LV as reference for comparison. Asterisks indicate level of significant differences between CP technical mixtures: $p \leq 0.05$ (*); $p \leq 0.01$ (**); $p \leq 0.001$ (***).

	Estimate	SE	t-value	p-value
Cereclor S45	-0.4	0.04	-9.6	***
CP-52	0.05	0.03	1.5	0.16
Huels 70C	0.04	0.04	1.2	0.27

Table S13. Linear regressions (y = ax + b) for the relationships between chlorine content and between log $K_{silicone\text{-}water}$ and log $K_{oc\text{-}water}$. P-value describes how good is chlorine as a predictor to the response variables (log $K_{silicone\text{-}water}$ and log $K_{oc\text{-}water}$). Asterisks indicate level of significance for the slope (a): $p \leq 0.05$ (*); $p \leq 0.01$ (**); $p \leq 0.001$ (***).

	a	b	df	R^2	p
log $K_{silicone\text{-}water}$	0.032	0.008	85	0.17	***
log $K_{oc\text{-}water}$	0.058	0.014	43	0.28	**

Table S14. Total CP body burden. DW of juvenile *D. magna* after 48 h exposure. concentration in water of each CP mixture. immobilization observed in the Acute Immobilization Test (OECD 202 guidelines) for the control (n=15). blanks (n=15) and treatments (n=5). Values are shown as mean ± SD. P-value shows the difference between immobilization for different treatments, when compared to the control. Asterisks indicate level of significance: $p \leq 0.05$ (*); $p \leq 0.01$ (**); $p \leq 0.001$ (***).

	DW daphnid / µg	Coc / ng/µg OC	Cwater / µg/L	Immobilization / %
Control	4.1 ± 2.1	0	0	2 ± 0.04
Blanks	8.0 ± 2.7	0	0	0
Cereclor 50LV	7.2 ± 1.9	89.5±31.0	40±8	0
	7.6 ± 1.3	50.6±35.2	50±11	10 ± 7*
Cereclor S45	5.8 ± 3.1	41.8±24.9	70±30	2 ± 4
	6.3 ± 1.6	32.64±9.1	120±7.5	4 ± 5
	7.2 ± 1.9	60.0±42.37	260±11	12 ± 8 *
CP-52	6.2 ± 1.3	72.1±17.2	23±4.7	4 ± 5
	6.18*	25.9±3.9	100±11	4 ± 5
	6.18*	141.7±84.2	280±18	36 ± 11***

*Dry weight was not measured for this treatment. Therefore the mean observed value was used.