# Supporting Information - Bioaccumulation potential of CPs in aquatic organisms: Uptake and depuration in *Daphnia magna*

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## Calculation of modelled log BAF values

Modelled log BAF values were obtained using U.S. Environmental Protection Agency's $K_{ow}$ (based) Aquatic Bioaccumulation Model (KABAM version 1.0 (2009))*, which is based on an aquatic food web bioaccumulation model published by Arnot and Gobas.[1] The model was adapted for filter feeders.

For the calculation of the modelled BAF value, the $K_{ow}$ input value (T=20°C) was for each mixture was estimated using the US EPA EPISuite software package (version 4.1) predicted by KOWWIN and BCFBAF tools. The $K_{ow}$ was calculated for 224 congeners (from $C_9Cl_3$ to $C_{31}Cl_{12}$). For each molecular formula, one isomer was selected with the following assumptions: i) equally distributed chlorine substitution through the carbon chain starting from the middle of the chain and ii) one chlorine per carbon atom. The reconstructed congener composition of each CP technical mixture was used to calculate the relative contribution (RC) of each congener in the whole mixture, which multiplied by each congener specific $K_{ow}$, gave a final estimated $K_{ow}$ (Equation (S1)).

$$K_{ow}(estimated) = \sum K_{ow_{congener1}} \times RC_{congener1} + \ldots + K_{ow_{congener\,n}} \times RC_{congener\,n} \quad \text{(S1)}$$

Feeding rate was measured through a simple 24 hour feeding test, instead of modelled through KABAM. The feeding test performed in this work was done according to Barata et al. (2008), where feeding rate was measured with an initial food concentration of 4 μg C $mL^{-1}$. Feeding rate of the animals (model input value) was $7.7\times10^{-7}$ kg algae $day^{-1}$.

*https://www.epa.gov/pesticide-science-and-assessing-pesticide-risks/kabam-version-10-users-guide-and-technical-7#A2

**Table S1.** Average recoveries (%) obtained for water and daphnia samples for the different CP mixtures.

| | Cereclor S45 | Cereclor 50LV | Huels 70C | CP-42 | CP-52 | Overall average |
|---|---|---|---|---|---|---|
| Water samples | 144 ± 43 | 100 ± 24 | 89 ± 19 | 73 ± 22 | 88 ± 15 | 101 |
| Daphnia samples | 172 ± 57 | 151 ± 70 | 99 ± 26 | 125 ± 28 | 139 ± 37 | 130 |

**Table S2.** Comparison between modelled (mod.) and experimental (exp.) log BAF (L kg lip$^{-1}$) for the CP technical mixtures used in this study, as well as estimated rate constants for uptake through diet ($k_F$, kg food kg organism day$^{-1}$), uptake through respiration ($k_1$, L kg day$^{-1}$), elimination through respiration ($k_2$, day$^{-1}$), elimination through excretion of feces ($k_E$, day$^{-1}$), growth ($k_G$, day$^{-1}$) and metabolism ($k_M$, day$^{-1}$). Concentration of CPs in water ($C_{water}$ (exp.), g L$^{-1}$) input values were obtained from this study, and used for the calculation of the concentration of CPs in *D. magna* originating from uptake through respiration ($C_{D.magna}$ (respiration), g kg ww$^{-1}$). Concentration of CPs in *D. magna* originating from uptake through diet ($C_{D.magna}$ (diet), g kg ww$^{-1}$) was estimated from the concentration of CPs in algae, in turn estimated from the $K_{oc\text{-}water}$ calculated for these mixtures in a previous study [3] and concentrations in water quantified in this study, using 50% organic carbon content (Table S3). $C_{D.magna}$ (g kg ww$^{-1}$) was calculated as according to KABAM version 1.0 (2009), from the different rate constants. Non-listed parameters were calculated as described in KABAM version 1.0 (2009). Other parameter values can be found in Table S4. References for the different values used are indicated within parenthesis.

| | Cereclor S45 | Cereclor 50LV | Huels 70C | CP-42 | CP-52 | PCB-138 | PCB-180 |
|---|---|---|---|---|---|---|---|
| **log BAF (exp.)** | **6.7** | **6.9** | **7.0** | **6.5** | **7.0** | **7.30 (4)** | **7.25 (4)** |
| **log BAF (mod.)** | **6.9** | **6.5** | **7.4** | **7.0** | **7.6** | **8.1** | **8.7** |
| log $K_{ow}$ | 7.88 | 6.24 | 7.03 | 9.79 | 8.07 | 6.83 | 7.36 |
| $C_{water}$ (exp.) | $1.2\times10^{-6}$ | $2.3\times10^{-6}$ | $5.8\times10^{-7}$ | $1.4\times10^{-6}$ | $1.4\times10^{-6}$ | $7.5\times10^{-13}$ (4) | $2.3\times10^{-13}$ (5) |
| $C_{D.magna}$ | 0.67 | 0.49 | 1.07 | 0.87 | 3.6 | $5.8\times10^{-6}$ | $8\times10^{-6}$ |
| $C_{D.magna}$ (diet) | 0.04 | 2.2 | 0.9 | 0.00057 | 0.37 | $7.6\times10^{-6}$ (5) | $3.5\times10^{-6}$ (5) |
| $C_{D.magna}$ (respiration) | 0.008 | 0.2 | 0.04 | 0.05 | 0.09 | $5\times10^{-8}$ | $1.5\times10^{-8}$ |
| $k_1$ | $6.6\times10^{4}$ | $6.6\times10^{4}$ | $6.6\times10^{4}$ | $6.6\times10^{4}$ | $6.6\times10^{4}$ | $6.6\times10^{4}$ | $6.6\times10^{4}$ |
| $k_F$ | 0.12 | 1.2 | 0.6 | 0.002 | 0.08 | 0.76 | 0.34 |
| $k_2$ | 0.11 | 4.7 | 0.76 | 0.001 | 0.07 | 1.2 | 0.36 |
| $k_E$ | 0.01 | 0.10 | 0.05 | 0.00014 | 0.007 | 0.06 | 0.03 |
| $k_G$ | 0.04 | 0.04 | 0.04 | 0.04 | 0.04 | 0.04 | 0.04 |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| $k_M$ | 0 | 0 | 0 | 0 | 0 | 0 | 0 |

**Table S3.** log $K_{oc\text{-}water}$ considered for the calculation of concentration of CPs in algae, used to estimate the concentration of CPs in *D. magna* originating from uptake through diet ($C_{D.magna}$ (diet), g kg $ww^{-1}$) in Table S2. References for the different values used are indicated within parenthesis.

| CP substance | log *K*oc | $C_{algae}$ (g/kgww) | $C_{D.magna}$ (diet) |
|---|---|---|---|
| Cereclor S45 | 5.73(3) | 0.29 | 0.04 |
| Cereclor 50LV | 6.24(3) | 1.8 | 2.2 |
| Huels 70C | 6.76(3) | 1.5 | 0.9 |
| CP-42 | 5.73* | 0.34 | 0.00057 |
| CP-52 | 6.3(3) | 2.1 | 0.37 |
| PCB-138 | - | $1.0\times10^{-5}$ (5) | $7.6\times10^{-6}$ |
| PCB-180 | - | $1.0\times10^{-5}$ (5) | $3.6\times10^{-6}$ |

*not measured in Castro et al., 2018, assumed to be closest to that of Cereclor S45

**Table S4.** Values used for the different physical-chemical and biological parameters used in the KABAM model, necessary to most accurately model log BAF (L kg $lip^{-1}$, Table S2).

| Parameter | Value | Unit | Reference |
|---|---|---|---|
| Concentration of dissolved $O_2$ | 8 | mg/L | Measured |
| Temperature | 20 | °C | Standard |
| Total organic carbon in water | $2\times10^{-9}$ | kg/L | Measured |
| Fraction of diet containing the chemical | 100 | % | |
| Algae cell dry weight | $1.42\times10^{-14}$ | kg | [6] |
| Algae cell water content | 94.64 | % | [7]* |
| Algae cell wet weight | $2.7\times10^{-13}$ | kg | [6,7] |
| Algae cell organic carbon (dw) | 50 | % | |
| Algae cell organic carbon | $7.1\times10^{-15}$ | kg | |
| *D. magna* dry weight | $2.5\times10^{-8}$ | kg | This work** |
| *D. magna* water content | 90 | % | This work** |
| *D. magna* wet weight | $2.5\times10^{-7}$ | kg | This work** |
| *D. magna* lipid content (dw) | 7 | % | This work** |
| *D. magna* lipid content | $1.75\times10^{-8}$ | kg | This work** |
| *D. magna* organic carbon (dw) | 38.5 | % | [3] |
| *D. magna* organic carbon | $9.6\times10^{-7}$ | kg | [3] |

*value for *Desmodesmus sp*., same order as *P.subcapitata*.
** values obtained for a fed juvenile *D. magna* (3-4 days old), as used in this study.

References


(1) Arnot, J. A.; Gobas, F. A. P. C. A food web bioaccumulation model for organic chemicals in aquatic ecosystems. *Environ. Toxicol. Chem.* **2004**, *23* (10), 2343–2355.

(2) Barata, C.; Alañon, P.; Gutierrez-Alonso, S.; Riva, M. C.; Fernández, C.; Tarazona, J. V. A Daphnia magna feeding bioassay as a cost effective and ecological relevant sublethal toxicity test for Environmental Risk Assessment of toxic effluents. *Sci. Total Environ.* **2008**.

(3) Castro, M.; Breitholtz, M.; Yuan, B.; Athanassiadis, I.; Asplund, L.; Sobek, A. Partitioning of Chlorinated Paraffins (CPs) to Daphnia magna Overlaps between Restricted and in-Use Categories. *Environ. Sci. Technol.* **2018**, *52* (17), 9713–9721.

(4) Sobek, A.; McLachlan, M. S.; Borgå, K.; Asplund, L.; Lundstedt-Enkel, K.; Polder, A.; Gustafsson O, Ö. A comparison of PCB bioaccumulation factors between an arctic and a temperate marine food web. *Sci. Total Environ.* **2010**, *408* (13), 2753–2760.

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(6) Bossuyt, B. T. A.; Janssen, C. R. Long-term acclimation of Pseudokirchneriella subcapitata (Korshikov) Hindak to different copper concentrations: Changes in tolerance and physiology. *Aquat. Toxicol.* **2004**.

(7) Li, Z.; Li, Y.; Zhang, X.; Tan, T. Lipid extraction from non-broken and high water content microalgae Chlorella spp. by three-phase partitioning. *Algal Res.* **2015**.

**Figure S1.** Equilibration time for CP-52 in *D.magna*, using passive dosing. Concentrations of CP-52 (ng µg $dw^{-1}$) were measured after 24, 48 and 72 hours of contact time between dosed silicone, dosed water and *D. magna* (<3 days old).

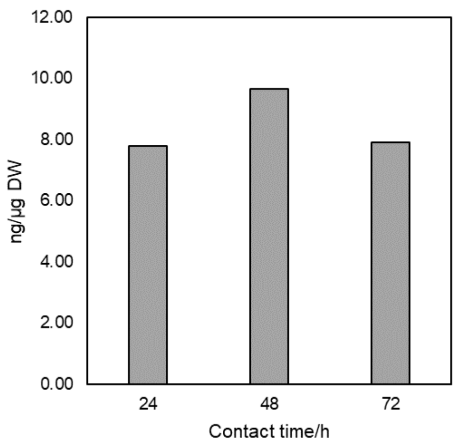

**Figure S2.** Depuration expressed as decrease in concentration in *D. magna* (compared to initial concentration at t=0; $C_{D.magna}$) versus time (*t* ), based on the calculated first order kinetic depuration rate constants for Cereclor 50LV (A), Huels 70C (B), Cereclor S45 (C), CP-52 (D) and CP-42 (E) with clean food and water (yellow, ▲) vs no food, just clean water (blue, ●).

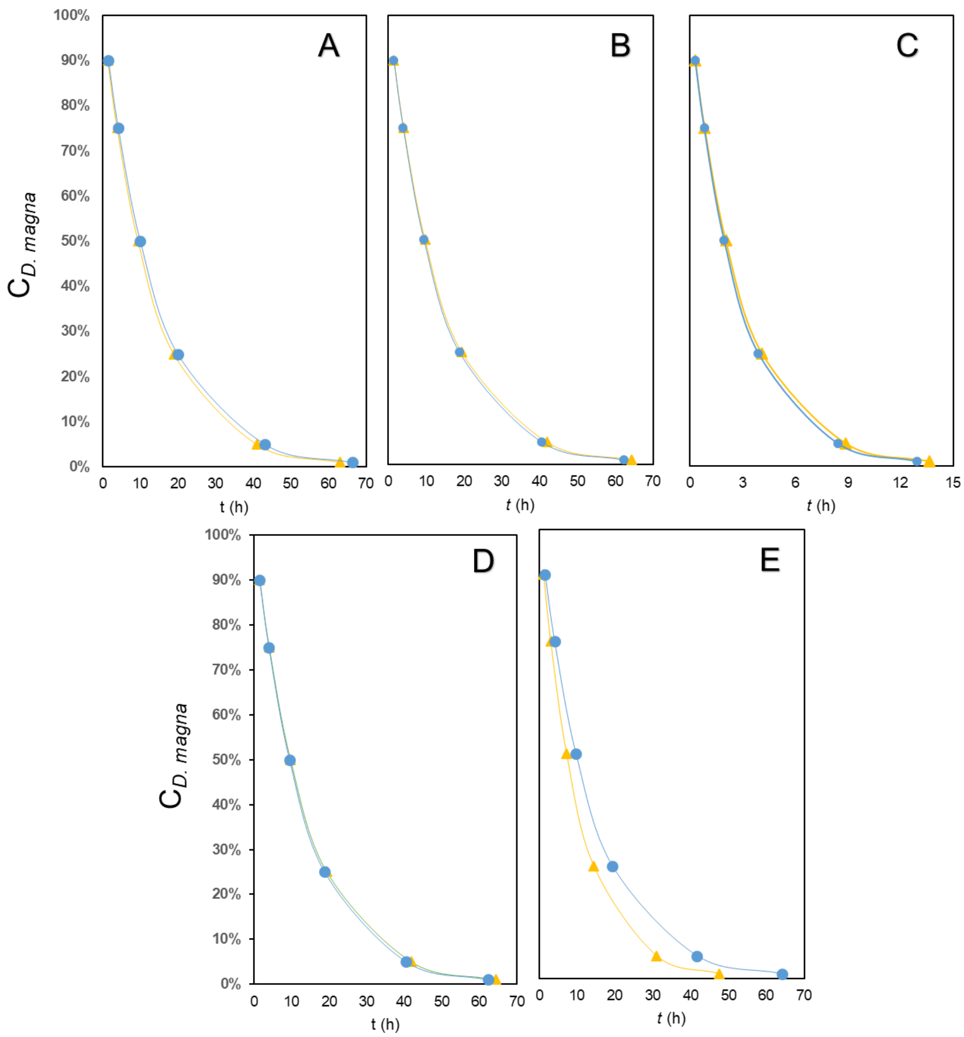

**Figure S3**. Visualization of the depuration progress calculated from the depuration rate constant (y axis, % $C_{D.magna}$) for the five different CP technical substances in *D. magna* over time (x axis, *t* (hours)). Cereclor S45 (■), Cereclor 50LV (×), CP-42 (+), Huels 70C (●) and CP-52 (▲).

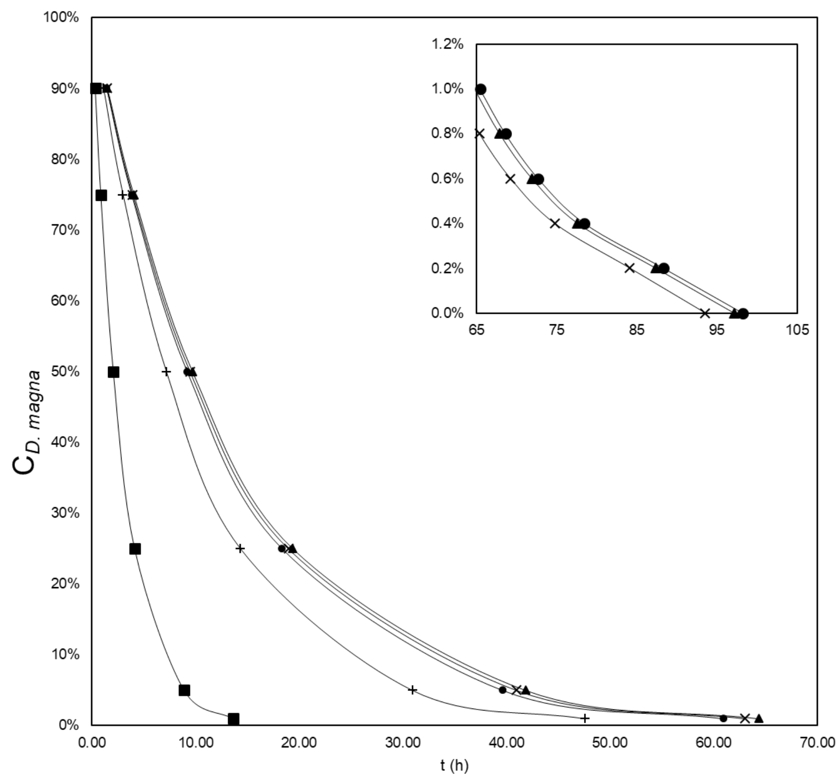

**Table S5.** Generalized linear models testing effects of the different CP mixtures on log BCF, using Cereclor 50LV and Huels 70C (SCCPs) as references for comparison.

| **Cereclor 50LV vs** | Estimate | SE | t-value | p-value |
|---|---|---|---|---|
| CP-42 | -0.06011 | 0.021 | -2.865 | 0.00832 |
| Cereclor S45 | -0.03113 | 0.021 | -1.495 | 0.14749 |
| CP-52 | -0.00494 | 0.021 | -0.237 | 0.815 |
| Huels 70C | 0.01812 | 0.021 | 0.881 | 0.38679 |
| **Huels 70C vs** | | | | |
| CP-42 | -0.07823 | 0.021 | -3.745 | 0.000950 |
| Cereclor S45 | -0.04925 | 0.021 | -2.375 | 0.025516 |
| Cereclor 50LV | -0.01812 | 0.021 | -0.881 | 0.386788 |
| CP-52 | -0.0231 | 0.021 | -1.110 | 0.27738 |

**Table S6.** Generalized linear models testing effects of the different CP mixtures on log BAF, using Cereclor 50LV and Huels 70C (SCCPs) as references for comparison.

| **Cereclor 50LV vs** | Estimate | SE | t-value | p-value |
|---|---|---|---|---|
| CP-42 | -0.047326 | 0.011 | -4.260 | 0.000254 |
| Cereclor S45 | -0.019306 | 0.011 | -1.750 | 0.092377 |
| CP-52 | 0.0214 | 0.011 | 1.966 | 0.061 |
| Huels 70C | 0.034898 | 0.011 | 3.206 | 0.003657 |
| **Huels 70C vs** | | | | |
| CP-42 | -0.082224 | 0.011 | -7.463 | 8.13e-08 |
| Cereclor S45 | -0.054203 | 0.011 | -4.956 | 4.18e-05 |
| Cereclor 50LV | -0.034898 | 0.011 | -3.206 | 0.0037 |
| CP-52 | -0.0135 | 0.011 | -1.253 | 0.222 |

**Table S7.** Two sample t-test comparison of the log BCF and log BAF obtained for the different CP technical mixtures.

| | t-value | df | p-value |
|---|---|---|---|
| Cereclor S45 | 3.2785 | 5 | 0.02199 |
| Cereclor 50LV | 5.1325 | 5 | 0.003668 |
| Huels 70C | 1.9095 | 5 | 0.1145 |
| CP-42 | 2.7683 | 5 | 0.03945 |
| CP-52 | 3.7928 | 5 | 0.0127 |

**Table S8.** Linear regressions (y = ax + b) for the relationships between chlorine content and between log BCF and BAF. The p-value describes how good chlorine is as a predictor for the response variables (log BCF and log BAF).

| | a | b | df | $R^2$ | p |
|---|---|---|---|---|---|
| log BCF | 0.0167 | 0.005 | 28 | 0.27 | 0.00215 |
| log BAF | 0.0177 | 0.003 | 28 | 0.54 | $2.06\times10^{-6}$ |

**Table S9.** Generalized linear models testing effects using CP-42 as reference the different log BCF and BAF values obtained for the different substances, used for Figure 2.

**BCF comparison**

| CP-42 vs | Estimate | SE | t-value | p-value |
|---|---|---|---|---|
| Cereclor S45 | 0.029 | 0.21 | 1.360 | 0.186 |
| Cereclor 50LV | 0.06 | 0.2115 | 2.842 | 0.00879 |
| CP-52 | 0.0552 | 0.0212 | 2.606 | 0.01523 |
| Huels 70C | 0.07823 | 0.0211 | 3.715 | 0.00103 |

**BAF comparison**

| CP-42 vs | | | | |
|---|---|---|---|---|
| Cereclor S45 | 0.028 | 0.0111 | 2.520 | 0.019 |
| Cereclor 50LV | 0.047 | 0.0111 | 4.276 | 0.000243 |
| CP-52 | 0.0687 | 0.0110 | 6.240 | $1.58\times10^{-6}$ |
| Huels 70C | 0.0822 | 0.0110 | 7.492 | $7.61\times10^{-8}$ |

**Figure S4**. Congener pattern observed in *D. magna* after Cereclor 50LV aqueous exposure (top) and original CP pattern of Cereclor 50LV (bottom). Similarity between patterns was >84 using the goodness of fit ($R^2$) between the pattern of the technical mixture and that of the sample.

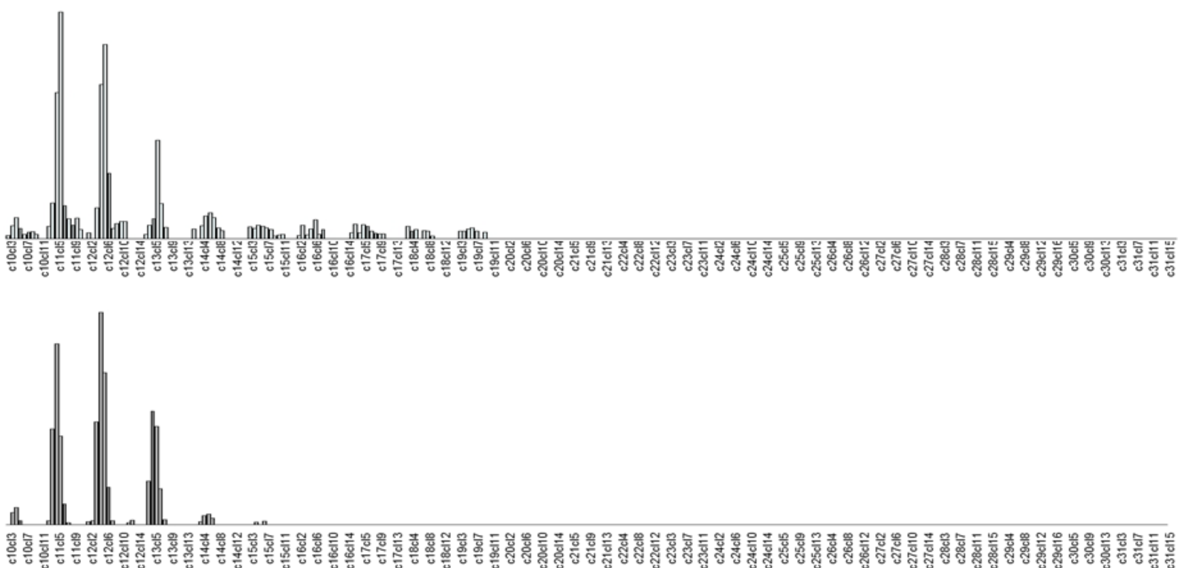

**Figure S5**. Congener pattern observed in *D. magna* after Huels 70C aqueous exposure (top) and original CP pattern of Huels 70C (bottom). Similarity between patterns was >95 using the goodness of fit ($R^2$) between the pattern of the technical mixture and that of the sample.

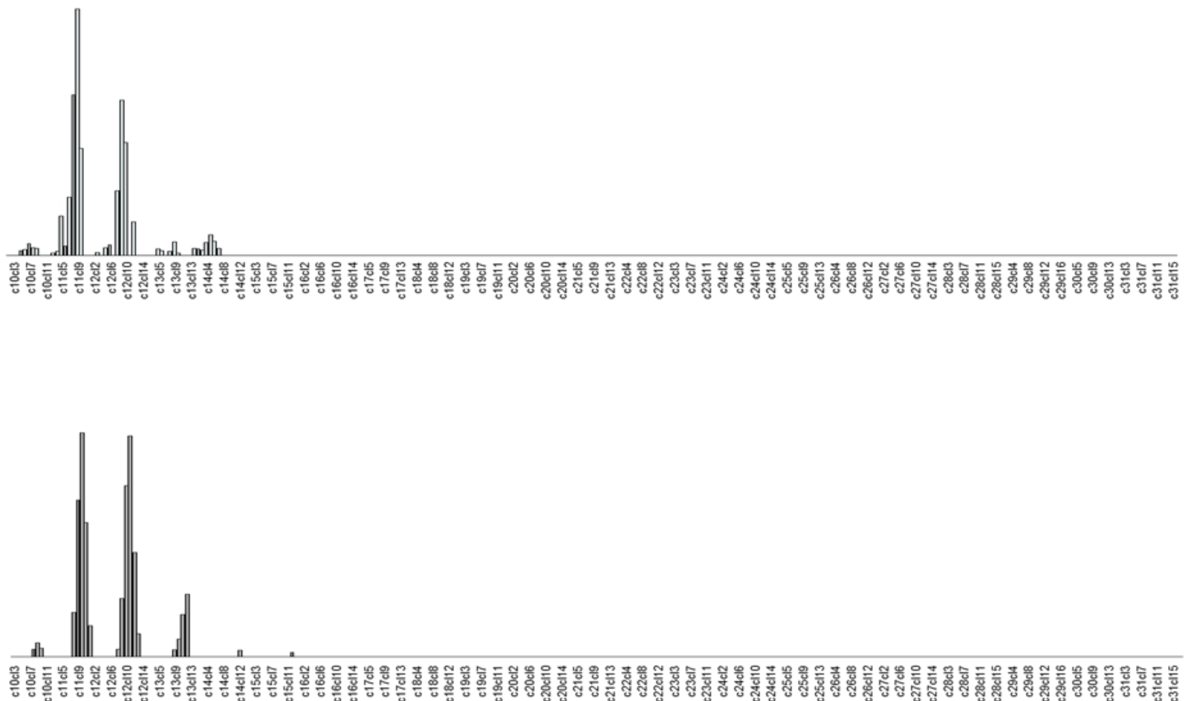

**Figure S6**. Congener pattern observed in *D. magna* after Cereclor S45 aqueous exposure (top) and original CP pattern of Cereclor S45 (bottom). Similarity between patterns was >90 using the goodness of fit ($R^2$) between the pattern of the technical mixture and that of the sample.

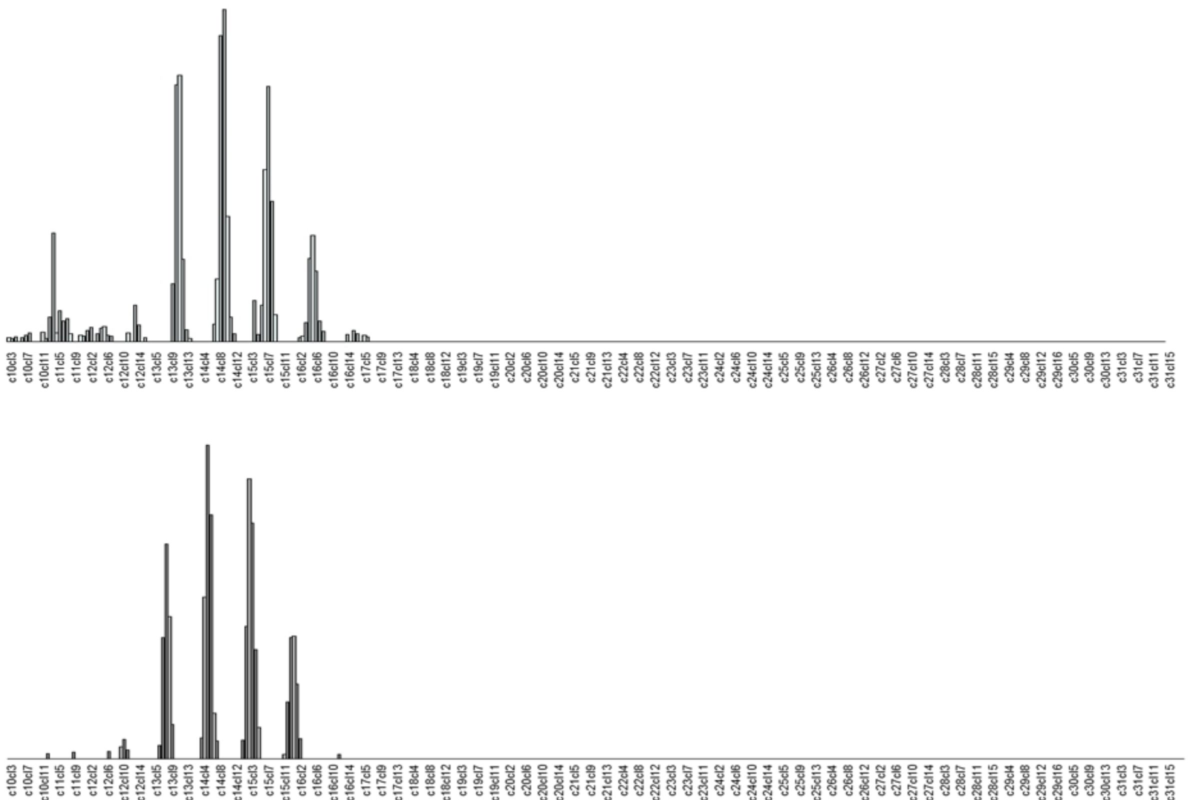

**Figure S7**. Congener pattern observed in *D. magna* after CP-52 aqueous exposure (bottom) and original CP pattern of CP-52 (top). Similarity between patterns was >80 using the goodness of fit ($R^2$) between the pattern of the technical mixture and that of the sample.

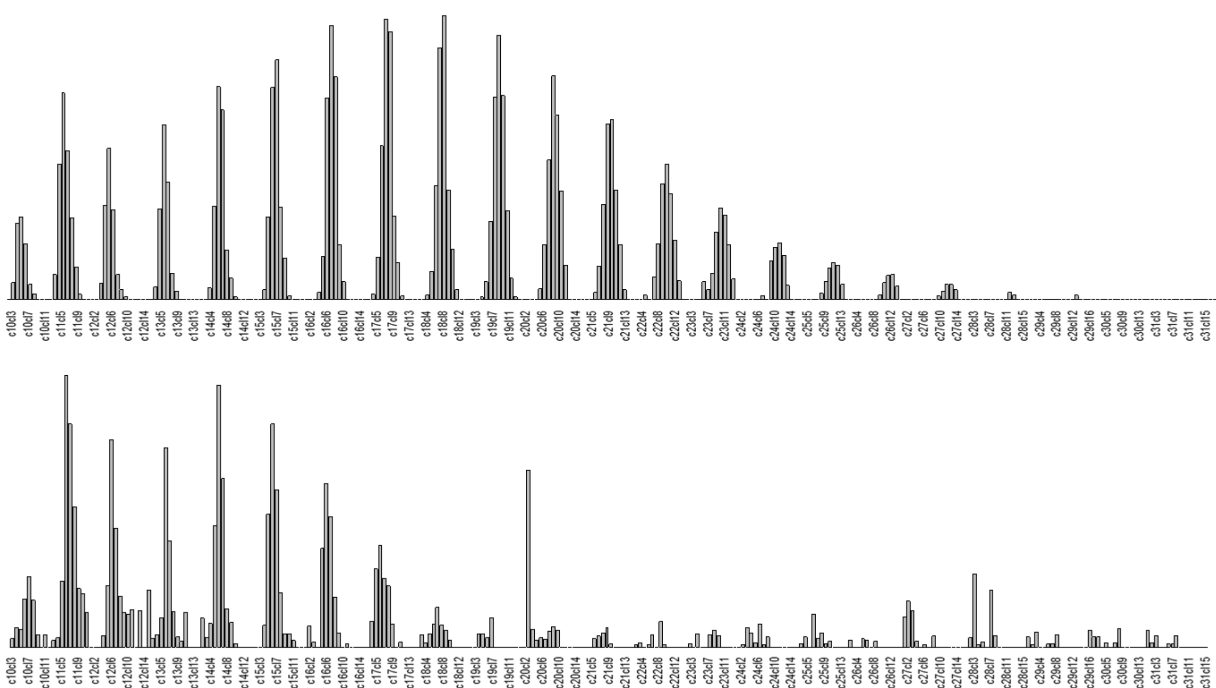

**Table S10**. List of congeners with molecular weight above 650 Da found in the original CP technical mixture and in exposed *D. magna*.

| | Cl% | MW | CP-42 | *D. magna* | CP-52 | *D. magna* |
|---|---|---|---|---|---|---|
| $C_{18}Cl_{12}$ | 64 | 667.84 | x | - | x | - |
| $C_{19}Cl_{12}$ | 62 | 681.86 | x | - | x | - |
| $C_{20}Cl_{11}$ | 59 | 661.44 | x | - | x | x |
| $C_{20}Cl_{12}$ | 61 | 695.89 | - | - | x | - |
| $C_{21}Cl_{10}$ | 55 | 641.02 | - | - | x | x |
| $C_{21}Cl_{11}$ | 58 | 675.47 | - | - | x | x |
| $C_{21}Cl_{12}$ | 60 | 709.91 | - | - | x | - |
| $C_{22}Cl_{10}$ | 54 | 655.05 | x | x | x | x |
| $C_{22}Cl_{11}$ | 57 | 689.50 | x | - | x | x |
| $C_{22}Cl_{12}$ | 59 | 723.94 | - | - | x | - |
| $C_{23}Cl_{10}$ | 53 | 669.08 | x | x | x | x |
| $C_{23}Cl_{11}$ | 55 | 703.52 | - | - | x | x |
| $C_{23}Cl_{12}$ | 58 | 737.97 | - | - | x | - |
| $C_{24}Cl_{10}$ | 52 | 683.10 | x | x | x | x |
| $C_{24}Cl_{11}$ | 54 | 717.55 | x | x | x | x |
| $C_{24}Cl_{12}$ | 57 | 751.99 | x | - | x | - |
| $C_{25}Cl_{9}$ | 48 | 662.69 | x | x | x | x |
| $C_{25}Cl_{10}$ | 51 | 697.13 | x | x | x | x |
| $C_{25}Cl_{11}$ | 53 | 731.58 | x | x | x | x |
| $C_{25}Cl_{12}$ | 56 | 766.02 | x | - | x | - |
| $C_{26}Cl_{9}$ | 47 | 676.71 | x | x | x | x |
| $C_{26}Cl_{10}$ | 50 | 711.16 | x | x | x | x |
| $C_{26}Cl_{11}$ | 52 | 745.60 | x | x | x | x |
| $C_{26}Cl_{12}$ | 55 | 780.05 | x | - | x | - |
| $C_{27}Cl_{8}$ | 43 | 656.29 | x | x | x | x |
| $C_{27}Cl_{9}$ | 46 | 690.74 | x | x | x | x |
| $C_{27}Cl_{10}$ | 49 | 725.18 | x | x | x | x |
| $C_{27}Cl_{11}$ | 51 | 759.63 | x | x | x | x |
| $C_{27}Cl_{12}$ | 54 | 794.07 | x | - | x | - |
| $C_{28}Cl_{8}$ | 42 | 670.32 | x | x | x | x |
| $C_{28}Cl_{9}$ | 45 | 704.77 | x | x | x | x |
| $C_{28}Cl_{10}$ | 48 | 739.21 | x | x | x | x |
| $C_{28}Cl_{11}$ | 50 | 773.66 | x | x | x | x |
| $C_{28}Cl_{12}$ | 53 | 808.10 | x | - | x | - |
| $C_{29}Cl_{8}$ | 41 | 684.35 | x | x | x | x |
| $C_{29}Cl_{9}$ | 44 | 718.79 | x | x | x | x |
| $C_{29}Cl_{10}$ | 47 | 753.24 | x | x | x | x |

| | | | | | | |
|---|---|---|---|---|---|---|
| $C_{29}Cl_{11}$ | 50 | 787.68 | x | x | x | x |
| $C_{29}Cl_{12}$ | 52 | 822.13 | x | - | x | - |
| $C_{30}Cl_{7}$ | 37 | 663.93 | x | x | x | x |
| $C_{30}Cl_{8}$ | 41 | 698.37 | x | x | x | x |
| $C_{30}Cl_{9}$ | 44 | 732.82 | x | x | x | x |
| $C_{30}Cl_{10}$ | 46 | 767.26 | x | x | x | x |
| $C_{30}Cl_{11}$ | 49 | 801.71 | x | - | x | x |
| $C_{30}Cl_{12}$ | 51 | 836.15 | - | - | x | x |
| $C_{31}Cl_{7}$ | 37 | 677.96 | x | x | x | x |
| $C_{31}Cl_{8}$ | 40 | 712.40 | x | x | x | x |
| $C_{31}Cl_{9}$ | 43 | 746.85 | x | x | x | x |
| $C_{31}Cl_{10}$ | 45 | 781.29 | x | x | x | x |
| $C_{31}Cl_{11}$ | 48 | 815.74 | x | x | x | - |
| $C_{31}Cl_{12}$ | 50 | 850.18 | x | - | x | - |

**Table S11.** List of congeners with log $K_{ow}$ above 12 found originally in the CP technical mixture and in exposed *D. magna*.

| | Cl% | log $K_{ow}$ | CP-42 | *D. magna* | CP-52 | *D. magna* |
|---|---|---|---|---|---|---|
| $C_{22}Cl_5$ | 37 | 12.05 | x | x | x | x |
| $C_{22}Cl_6$ | 41 | 12.23 | x | x | x | x |
| $C_{22}Cl_7$ | 45 | 12.41 | x | x | x | x |
| $C_{22}Cl_8$ | 48 | 12.59 | x | x | x | x |
| $C_{22}Cl_9$ | 51 | 12.77 | x | x | x | x |
| $C_{22}Cl_{10}$ | 54 | 12.95 | x | - | x | - |
| $C_{22}Cl_{11}$ | 57 | 13.13 | x | - | x | - |
| $C_{22}Cl_{12}$ | 59 | 13.31 | x | - | x | - |
| $C_{23}Cl_2$ | 18 | 12.00 | x | - | x | - |
| $C_{23}Cl_3$ | 25 | 12.18 | x | - | x | - |
| $C_{23}Cl_4$ | 31 | 12.36 | x | - | x | x |
| $C_{23}Cl_5$ | 36 | 12.54 | x | x | x | x |
| $C_{23}Cl_6$ | 40 | 12.72 | x | x | x | x |
| $C_{23}Cl_7$ | 44 | 12.9 | x | x | x | x |
| $C_{23}Cl_8$ | 47 | 12.59 | x | x | x | x |
| $C_{23}Cl_9$ | 50 | 13.26 | x | x | x | x |
| $C_{23}Cl_{10}$ | 53 | 13.44 | x | x | x | x |
| $C_{23}Cl_{11}$ | 55 | 13.62 | - | - | x | - |
| $C_{23}Cl_{12}$ | 58 | 13.8 | - | - | x | - |
| $C_{24}Cl_2$ | 17 | 12.49 | x | - | x | - |
| $C_{24}Cl_3$ | 24 | 12.67 | x | - | x | x |
| $C_{24}Cl_4$ | 30 | 12.85 | x | x | x | x |
| $C_{24}Cl_5$ | 35 | 13.03 | x | x | x | x |
| $C_{24}Cl_6$ | 39 | 13.21 | x | x | x | x |
| $C_{24}Cl_7$ | 43 | 13.39 | x | x | x | x |
| $C_{24}Cl_8$ | 46 | 13.57 | x | x | x | x |
| $C_{24}Cl_9$ | 49 | 13.75 | x | x | x | x |
| $C_{24}Cl_{10}$ | 52 | 13.93 | x | x | x | - |
| $C_{24}Cl_{11}$ | 54 | 14.11 | x | - | x | - |
| $C_{24}Cl_{12}$ | 57 | 14.29 | x | - | x | - |
| $C_{25}Cl_4$ | 29 | 13.34 | x | - | x | x |
| $C_{25}Cl_5$ | 34 | 13.52 | x | x | x | x |
| $C_{25}Cl_6$ | 38 | 13.7 | x | x | x | x |
| $C_{25}Cl_7$ | 42 | 13.88 | x | x | x | x |
| $C_{25}Cl_8$ | 45 | 14.06 | x | x | x | x |
| $C_{25}Cl_9$ | 48 | 14.24 | x | x | x | x |
| $C_{25}Cl_{10}$ | 51 | 14.42 | x | x | x | x |

| | | | | | | |
|---|---|---|---|---|---|---|
| $C_{25}Cl_{11}$ | 53 | 14.6 | x | x | x | - |
| $C_{25}Cl_{12}$ | 56 | 14.78 | x | - | x | - |
| $C_{26}Cl_{2}$ | 16 | 13.47 | x | - | x | - |
| $C_{26}Cl_{3}$ | 23 | 13.65 | x | - | x | x |
| $C_{26}Cl_{4}$ | 28 | 13.83 | x | x | x | x |
| $C_{26}Cl_{5}$ | 33 | 14.01 | x | x | x | x |
| $C_{26}Cl_{6}$ | 37 | 14.19 | x | x | x | x |
| $C_{26}Cl_{7}$ | 41 | 14.37 | x | x | x | x |
| $C_{26}Cl_{8}$ | 44 | 14.55 | x | x | x | x |
| $C_{26}Cl_{9}$ | 47 | 14.73 | x | x | x | x |
| $C_{26}Cl_{10}$ | 50 | 14.91 | x | x | x | - |
| $C_{26}Cl_{11}$ | 52 | 15.1 | x | x | x | - |
| $C_{26}Cl_{12}$ | 55 | 15.28 | x | - | x | - |
| $C_{27}Cl_{2}$ | 16 | 13.96 | x | - | x | x |
| $C_{27}Cl_{3}$ | 22 | 14.14 | x | - | x | x |
| $C_{27}Cl_{4}$ | 27 | 14.32 | x | - | x | x |
| $C_{27}Cl_{5}$ | 32 | 14.50 | x | x | x | x |
| $C_{27}Cl_{6}$ | 36 | 14.68 | x | x | x | x |
| $C_{27}Cl_{7}$ | 40 | 14.86 | x | x | x | x |
| $C_{27}Cl_{8}$ | 43 | 15.05 | x | x | x | x |
| $C_{27}Cl_{9}$ | 46 | 15.23 | x | x | x | x |
| $C_{27}Cl_{10}$ | 49 | 15.41 | x | x | x | - |
| $C_{27}Cl_{11}$ | 51 | 15.59 | x | x | x | - |
| $C_{27}Cl_{12}$ | 54 | 15.77 | x | - | x | - |
| $C_{28}Cl_{2}$ | 15 | 14.45 | x | - | x | - |
| $C_{28}Cl_{3}$ | 21 | 14.63 | x | - | x | - |
| $C_{28}Cl_{4}$ | 27 | 14.81 | x | x | x | x |
| $C_{28}Cl_{5}$ | 31 | 14.99 | x | x | x | x |
| $C_{28}Cl_{6}$ | 35 | 15.18 | x | x | x | x |
| $C_{28}Cl_{7}$ | 39 | 15.36 | x | x | x | x |
| $C_{28}Cl_{8}$ | 42 | 15.54 | x | x | x | x |
| $C_{28}Cl_{9}$ | 45 | 15.72 | x | x | x | x |
| $C_{28}Cl_{10}$ | 48 | 15.90 | x | x | x | - |
| $C_{28}Cl_{11}$ | 50 | 16.08 | x | x | x | - |
| $C_{28}Cl_{12}$ | 53 | 16.26 | x | - | x | - |
| $C_{29}Cl_{2}$ | 15 | 14.94 | x | - | x | - |
| $C_{29}Cl_{3}$ | 21 | 15.12 | x | - | x | x |
| $C_{29}Cl_{4}$ | 26 | 15.31 | x | - | x | x |
| $C_{29}Cl_{5}$ | 31 | 15.49 | x | x | x | x |
| $C_{29}Cl_{6}$ | 35 | 15.67 | x | x | x | x |
| $C_{29}Cl_{7}$ | 38 | 15.85 | x | x | x | x |
| $C_{29}Cl_{8}$ | 41 | 16.03 | x | x | x | x |
| $C_{29}Cl_{9}$ | 44 | 16.21 | x | x | x | x |
| $C_{29}Cl_{10}$ | 47 | 16.39 | x | x | x | - |

| | | | | | | |
|---|---|---|---|---|---|---|
| $C_{29}Cl_{11}$ | 50 | 16.57 | x | - | x | - |
| $C_{29}Cl_{12}$ | 52 | 16.75 | x | - | x | - |
| $C_{30}Cl_{2}$ | 14 | 15.44 | x | - | x | - |
| $C_{30}Cl_{3}$ | 20 | 15.62 | x | - | x | - |
| $C_{30}Cl_{4}$ | 25 | 15.80 | x | - | x | x |
| $C_{30}Cl_{5}$ | 30 | 15.98 | x | x | x | x |
| $C_{30}Cl_{6}$ | 34 | 16.16 | x | x | x | x |
| $C_{30}Cl_{7}$ | 37 | 16.34 | x | x | x | x |
| $C_{30}Cl_{8}$ | 41 | 16.52 | x | x | x | x |
| $C_{30}Cl_{9}$ | 44 | 16.70 | x | x | x | x |
| $C_{30}Cl_{10}$ | 46 | 16.88 | x | x | x | - |
| $C_{30}Cl_{11}$ | 49 | 17.06 | x | x | x | - |
| $C_{30}Cl_{12}$ | 51 | 17.24 | - | - | x | - |
| $C_{31}Cl_{2}$ | 14 | 15.93 | x | - | x | x |
| $C_{31}Cl_{3}$ | 20 | 16.11 | x | - | x | x |
| $C_{31}Cl_{4}$ | 25 | 16.29 | x | - | x | x |
| $C_{31}Cl_{5}$ | 29 | 16.47 | x | - | x | x |
| $C_{31}Cl_{6}$ | 33 | 16.65 | x | x | x | x |
| $C_{31}Cl_{7}$ | 37 | 16.83 | x | x | x | x |
| $C_{31}Cl_{8}$ | 40 | 17.01 | x | x | x | x |
| $C_{31}Cl_{9}$ | 43 | 17.19 | x | x | x | x |
| $C_{31}Cl_{10}$ | 45 | 17.37 | x | x | x | - |
| $C_{31}Cl_{11}$ | 48 | 17.55 | x | x | x | - |
| $C_{31}Cl_{12}$ | 50 | 17.73 | x | - | x | - |