Electronic Supplementary Material (ESI) for Environmental Science: Processes & Impacts

ELECTRONIC SUPPLEMENTARY INFORMATION

Evaluating the Environmental Fate of Short-Chain Chlorinated Paraffins (SCCPs) in the Nordic Environment Using a Dynamic Multimedia Model

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Table of Contents

1. Text

1.1 Details for the Emission Estimation Method

The high-throughput screening method is based on the EU Technical Guidance Document (TGD) on Risk Assessment,[1] and calculates the size of the emission and mode of entry (MOE) based on quantities in commerce, physical-chemical properties and chemical function information.[2] Experimental and estimated vapor pressures[3] and water solubilites[4-6] were used to divide the chemicals into bins that specify emission factors to air and water. However, the bins were too wide to differentiate between the SCCP formula groups. Input data on quantities in commerce for the years 2000-2007, broken down into categories of chemical function, were obtained from the SPIN-database (Substances in Preparations in Nordic Countries),[2] which contains information from the product registries of Norway, Sweden, Finland, and Denmark. Chemical function information is described by so-called Main Categories (MCs), Industrial Categories (ICs), and Use Categories (UC).[1] Estimations were made for multiple plausible IC/UC combinations as previously detailed, and emissions during production, formulation, industrial use, private use, and waste disposal were considered (with the product service life limited to one year).[7] For each individual year of 2000-2007, the IC/UC combination that yielded the lowest, average, and maximum emissions were identified, and the averages of the lowest, average, and maximum emissions over the 8 years were used as E_{MIN}, E_{AVG}, and E_{MAX}, respectively. When the emission estimates were scaled to the model domain, potential emissions in the tiny fractions of the Russian and German populations that are included in the model domain were ignored.

Ideally, the composition of the emissions is based on information about (i) the composition of all available technical mixtures, (ii) the relative production quantities of the technical mixtures, and (iii) chemical function for the various mixtures.[8] However, information on the relative production quantities and chemical function of the technical SCCPs mixtures is not available, and a simplified approach needs to be applied. A formula group profile for the emissions was based on an average between SCCPs with (i) 50-59 % and (ii) 60-70 % degree of chlorination. Average compositions for (i)-(ii) were based on the analysis of analytical standards and technical mixtures reported in the literature,[9-16] supplemented by results from routine analysis in our own laboratory (Table S5). The analytical standards that are used for quantification are produced by a similar free-radical chlorination process as the industrial technical mixtures,[e.g. 17,18] and are assumed to be representative for commercial SCCPs products.

1.2 Monte Carlo Uncertainty Analysis

For comparison to the analytical uncertainty analysis based on model sensitivity and confidence factors (*Cf*), a Monte Carlo analysis was performed for $\mathrm{SCCP}_{\mathrm{average}}$. To make the results from the two uncertainty analyses comparable, the natural logarithm of the compound properties was used as the mean of the lognormal distributions, and the standard deviation σ of the lognormal distributions calculated as[19]

$$\sigma = \frac{1}{2}\ln Cf \qquad \text{[S1]}$$

One thousand random numbers were generated for each input parameter from the distributions using the R statistical software package,[20] and these were varied simultaneously in 1000 model simulations. Hence the Monte Carlo uncertainty analyses carried out here also assumes that all input parameters are log-normally distributed and that they are uncorrelated, but unlike the analytical approach carried out in the main part of the paper it makes no assumptions on the linearity of the model.

The contribution to variance (CV) for model outputs of $\text{SCCP}_{\text{average}}$ were compared, including concentrations in physical and biotic compartments and hazard criteria for persistence and long-range atmospheric transport (LRAT) (the percentage left in the environment ten years after emission stop ($M_{10\text{Y}}$), and the characteristic travel distance (L_A), respectively, see ESI section 1.3 below for details) (Figure S2). The results from the two methods were similar for all model outputs, which implies that the assumption of model linearity or near-linearity is a reasonable assumption for the current application of CoZMoMAN.

1.3 Hazard Evaluation and Benchmarking Against PCBs

1.3.1 Methods and Definitions

As emission estimates are normally the largest source of uncertainty to risk evaluations, benchmarking studies where the hazard of chemicals is assessed independent of quantities facilitates comparison of contaminants based solely on their compound properties.[21,22] For comparison to the SCCPs, seven selected PCBs (PCB 28, 52, 101, 118, 138, 153 and 180) were included in the simulations with physical-chemical properties previously compiled from the literature by Breivik et al.[23] The same MOE for the emissions was used for the PCBs as for the SCCPs. The persistence, LRAT, and bioaccumulation of the PCBs and SCCPs were compared. As CoZMoMAN is a dynamic model which facilitates an analysis of the environmental response to changes in emissions in time, persistence was calculated as the percentage left in the physical environment 10 years after a hypothetical complete emission stop (M_{10Y}). LRAT was estimated as the characteristic travel distance (L_A), i.e. the distance it takes for the concentration in air to decrease to ≈ 37 % (1/e) of the initial concentration,[24,25] and bioaccumulation was illustrated with the concentration in a 29 year old female following 70 years of constant emissions (C_{fem29}).

1.3.2 Persistence

The estimated overall environmental persistence (M_{10Y}) of SCCPs varied considerably between the formula groups (Figure S7). The lowest chlorinated formula groups were quickly degraded (M_{10Y} = 1 %), while the persistence of the highest chlorinated ones were comparable to the most persistent of the seven PCBs (PCB 101, 118, 138, 153, 180), with more than 60 % still remaining in the environment ten years after emission stop. However, the predicted persistence is very sensitive to the environmental *HL*s in soil and sediment (Table S7). This is illustrated by the very high persistence for $SCCP_{EU\text{-}RAR}$ which is higher than for any of the individual formula groups (Figure S7), precisely because of the long *HL*s assumed for SCCPs in these compartments in the EU RARs (Table S3).

1.3.3 Long-Range Atmospheric Transport

The SCCPs were estimated to display a lower LRAT than most of the PCBs, comparable to PCB-180, and L_A ranged from 3,000 to 14,000 km (Figure S7). The variation in LRAT with chlorination degree and chain-length was not straight-forward, but can be rationalized on the basis of two competing atmospheric removal processes (Figure S6). For most formula groups LRAT was limited by atmospheric degradation by hydroxyl radicals. As the chlorination degree increases, LRAT was increasingly limited by deposition to surface media, and for $C_{12}H_{15}Cl_{11}$, $C_{13}H_{17}Cl_{11}$, and $C_{13}H_{16}Cl_{12}$ LRAT was only limited by deposition, similar to PCB-180 (Figure S6). Gawor and Wania[26] identified the most volatile SCCPs with up to 4 chlorines as “fliers” that have a low Arctic contamination potential (ACP) as they will not be effectively deposited to surface media. Similarly, they identified SCCPs with more than 9-10 chlorine atoms as “single hoppers” that are likely to be deposited prior to reaching the Arctic, and hence also have a low ACP, while SCCPs with an intermediate chlorination degree will be “multiple hoppers” with a higher ACP. The maximum ACP was predicted for SCCPs with 4 to 6 chlorine atoms, which also have a higher persistence in the atmosphere than the lower chlorinated ones, and hence could display a notable LRAT.[26] In this study the highest L_A was predicted for SCCPs with about 7-9 carbon atoms, hence with a higher degree of chlorination than by Gawor and Wania.[26] This is probably because atmospheric degradation is taken into account in the calculation of L_A but not in the estimation of ACP, even if it was subsequently qualitatively considered it in the interpretation of the ACP results.[26]

1.3.4 Bioaccumulation

With regard to bioaccumulation, the estimated concentration in a 29 year old female after 70 years of emissions (C_{fem29}) was considerably lower for most SCCPs compared to most PCBs (Figure S7), and the median C_{fem29} was 2.4 orders of magnitude higher for the PCBs than for $SCCP_{37}$. The predicted C_{fem29} for the SCCPs increased with increasing chain length and degree of chlorination, and the heaviest formula groups (C>10, Cl>8) displayed higher predicted C_{fem29} than PCB-28, PCB-52 and PCB-

101. This is similar to the findings in Gawor and Wania[26] where environmental bioaccumulation potential (EBAP) was found to increase with both the number of carbon and chlorine atoms, and SCCPs with less than 5-6 chlorines were located at the threshold for 10 % of maximum EBAP, indicating a low bioaccumulation potential in humans for these lower chlorinated SCCPs.

2. Figures

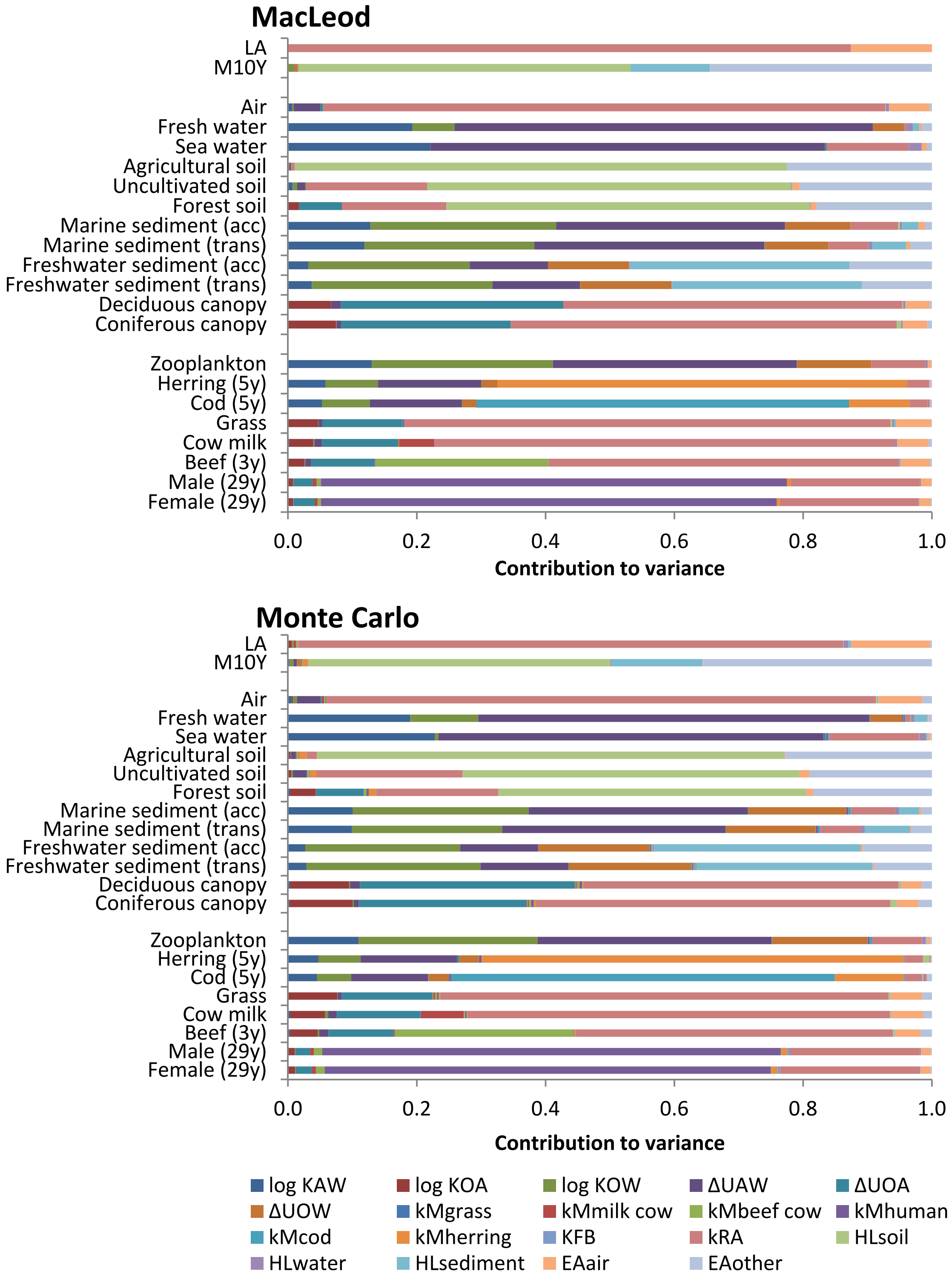

Figure S1: Contribution to variance for model outputs of SCCP$_{average}$ (LRAT (L_A), overall persistence (M_{10Y}) and concentrations in physical and biotic compartments) calculated from the analytical method (top) and the Monte Carlo method (bottom). Acc = accumulating, trans = transporting, and numbers in parentheses for the biotic compartments specify the age of the model organism in years.

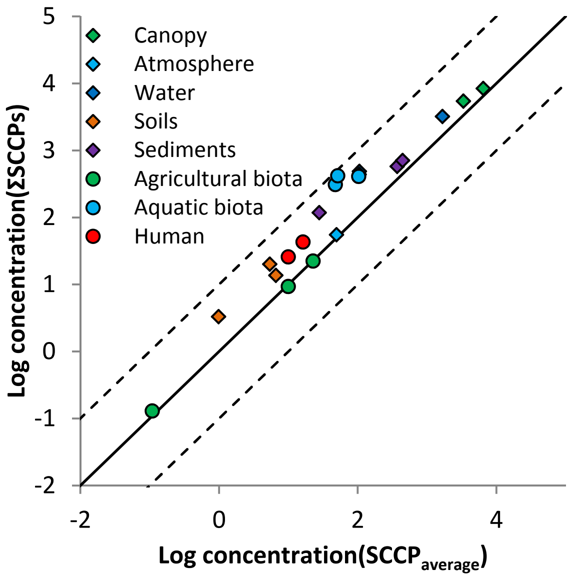

Figure S2: Comparison of the logarithm of the predicted ΣSCCPs concentrations based on all formula groups in the emission estimate against the logarithm of the predicted concentrations based on the average of the properties ($\mathrm{SCCP}_{\mathrm{average}}$). Both predictions are based on E_{MAX}. The solid line is the one-to-one line, while the dotted lines mark deviations of ± one order of magnitude.

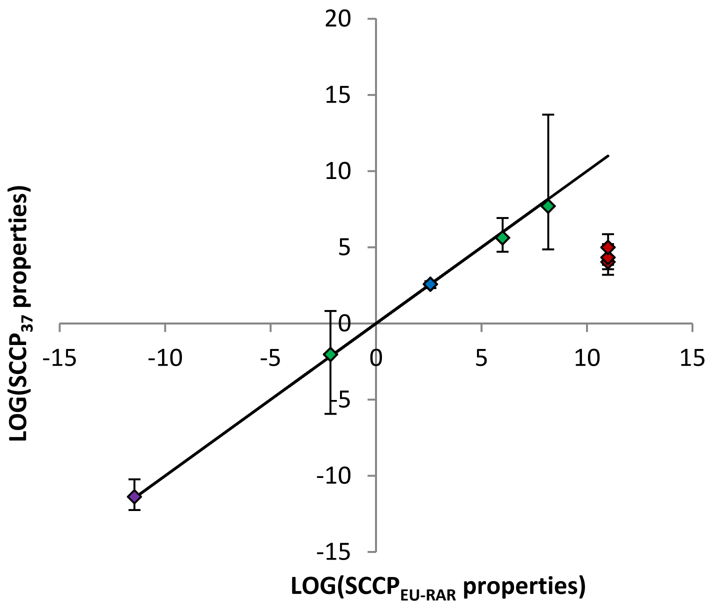

Figure S3: The median value and ranges of the logarithmic values of the molecular weight (blue), K_{OW}, K_{AW}, and K_{OA} (green), environmental *HL*s (red) and k_{RA} (purple) for SCCP_{37} against the same properties for $\mathrm{SCCP}_{\mathrm{EU\text{-}RAR}}$. The properties have various units. The kMs, *ΔU*s, K_{FB}, and *EA*s have not been included since they were not included in the EU RARs.[27,28]

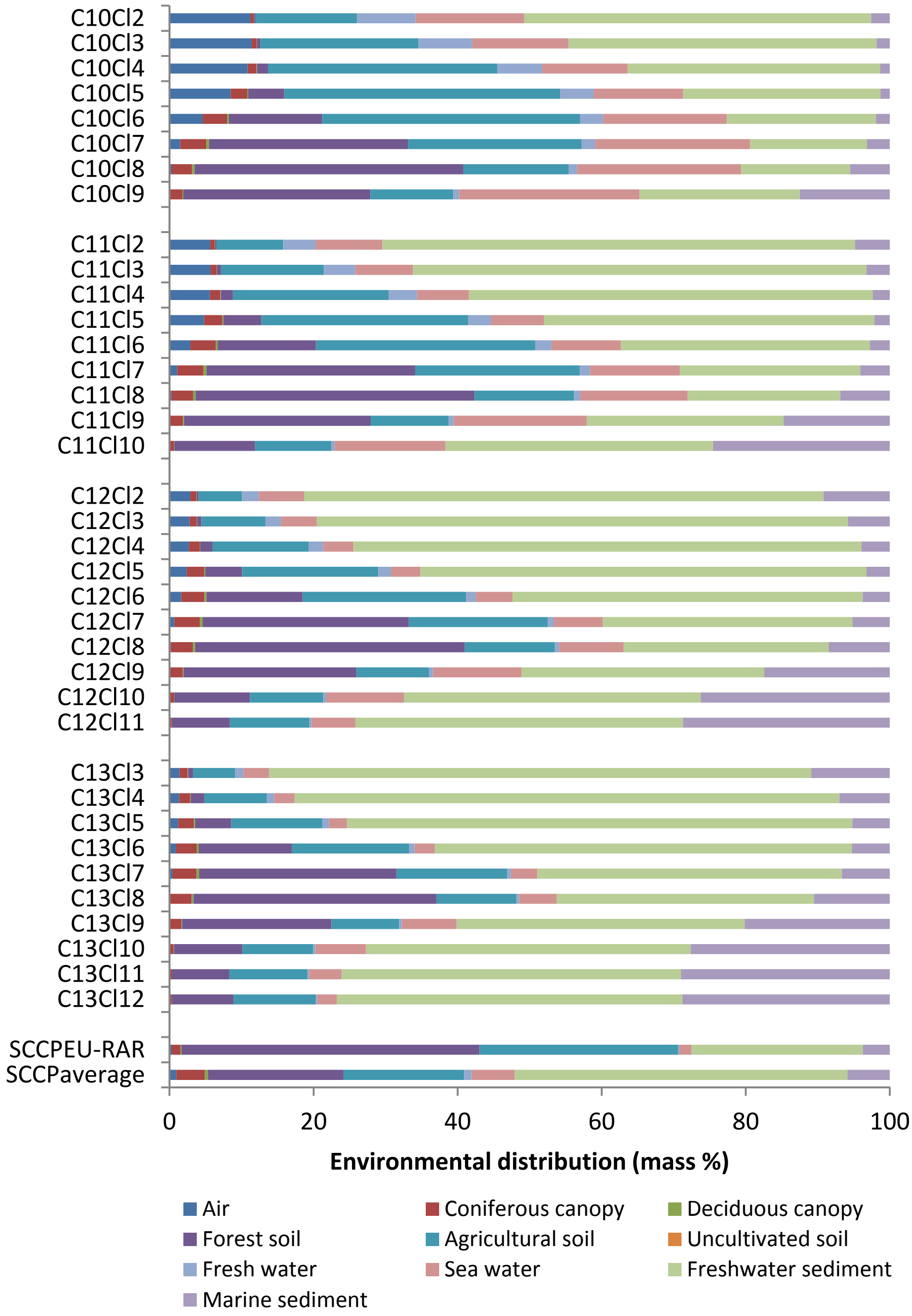

Figure S4: Environmental distribution, as percentage of total mass in the environment, for $SCCP_{37}$, $SCCP_{average}$, and $SCCP_{EU\text{-}RAR}$. The fractions in accumulating and transporting sediments have been added together.

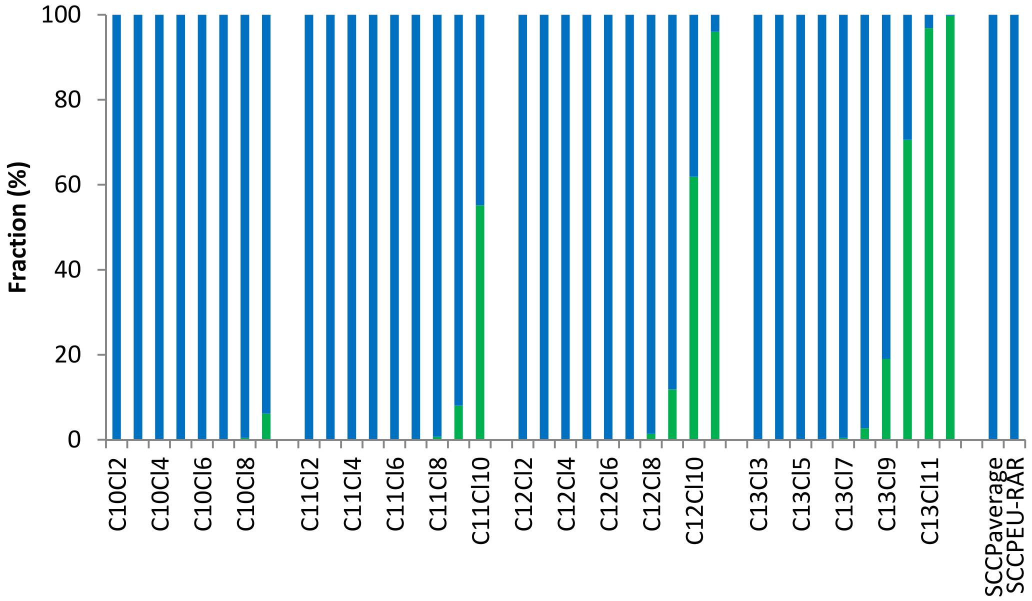

Figure S5: The annual average fraction that is estimated to be present in the gaseous phase (blue bars) or in the particulate phase (green bars) in the atmosphere for SCCP$_{37}$, SCCP$_{average}$, and SCCP$_{EU-RAR}$.

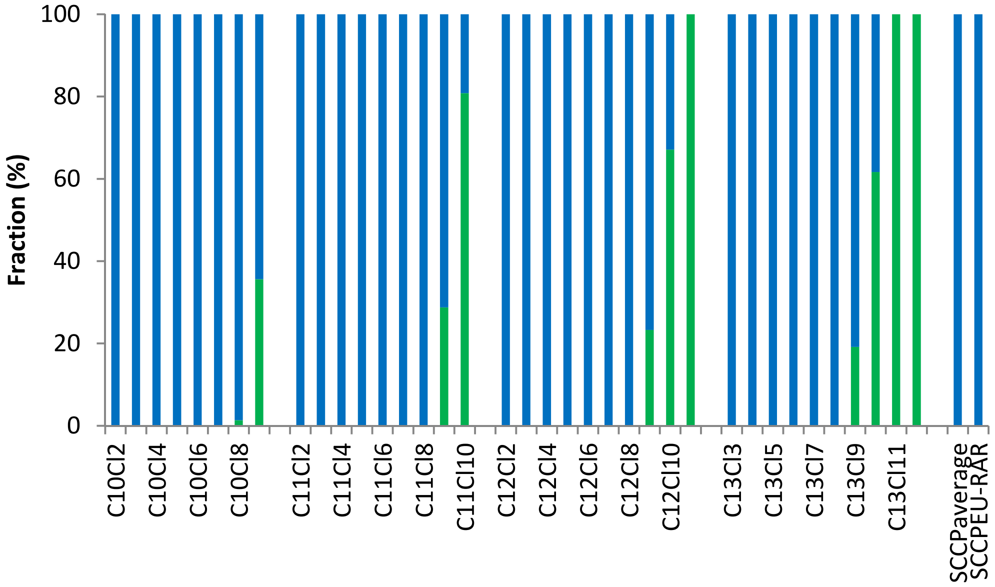

Figure S6: The fraction of times per year when the characteristic travel distance (*L_A*) is predicted to be limited by atmospheric degradation (blue bars) or deposition to surface media (green bars), relative to the total amount of stored events per year (*n* = 73), for SCCP$_{37}$, SCCP$_{average}$, and SCCP$_{EU-RAR}$.

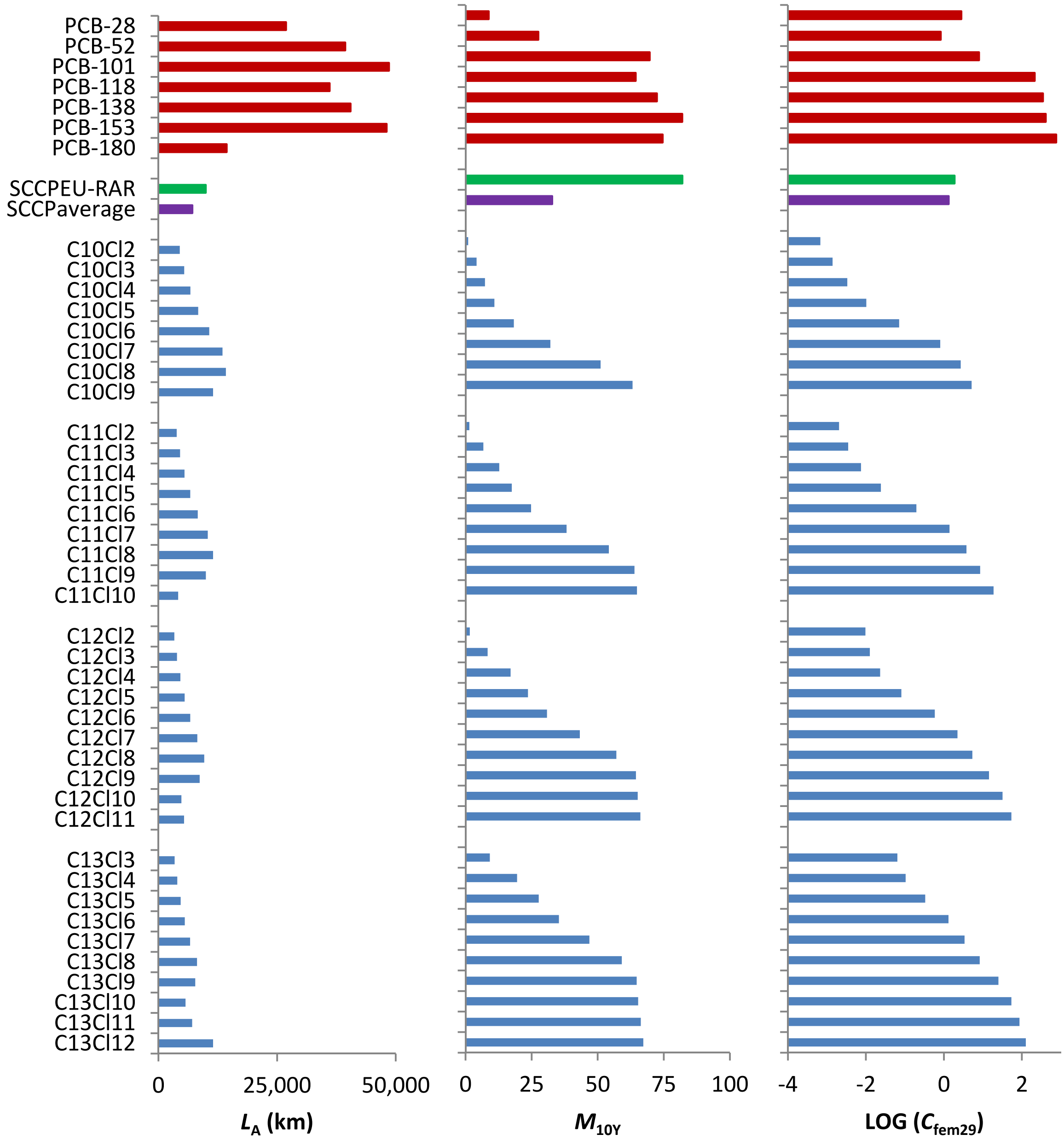

Figure S7: Benchmarking of SCCPs against PCBs. Results for the characteristic travel distance (L_A), overall persistence (M_{10Y}), and bioaccumulation (LOG(C_{fem29})) are displayed. Results are based on constant emissions for all formula groups, not incorporating the formula group composition of the emissions.

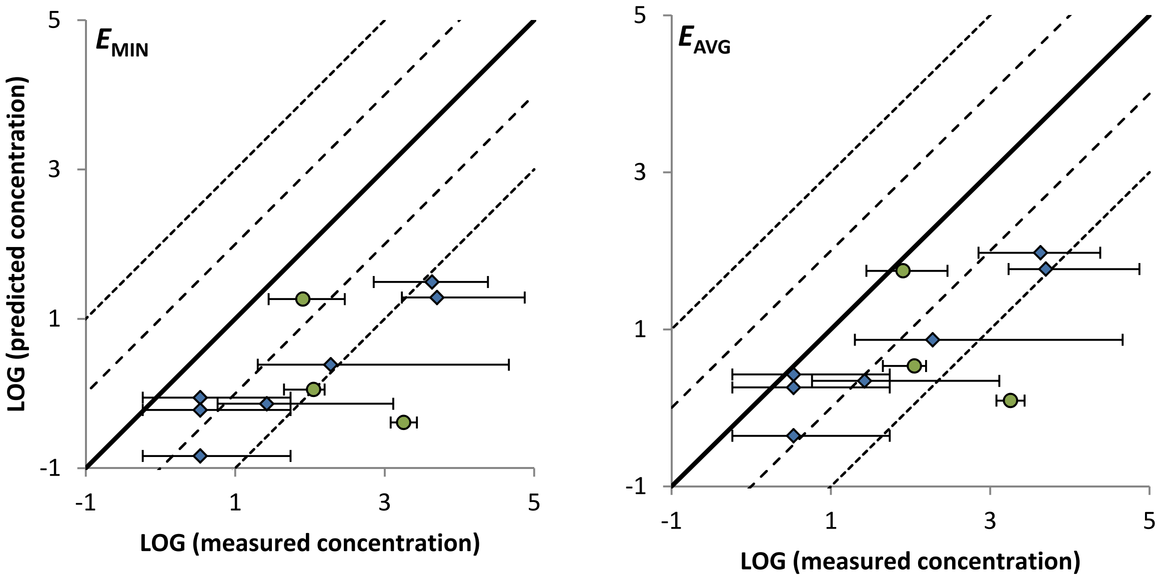

Figure S8: The logarithm of the predicted ΣSCCPs concentrations against the logarithm of the measured ΣSCCPs concentrations for the abiotic compartments (blue) and biota (green), based on the minimum (E_{MIN}) and average (E_{AVG}) emission estimates. The error bars show the ranges in the measured concentrations. The solid line is the one-to-one line, while the dotted lines mark deviations of ± 1 and 2 orders of magnitude.

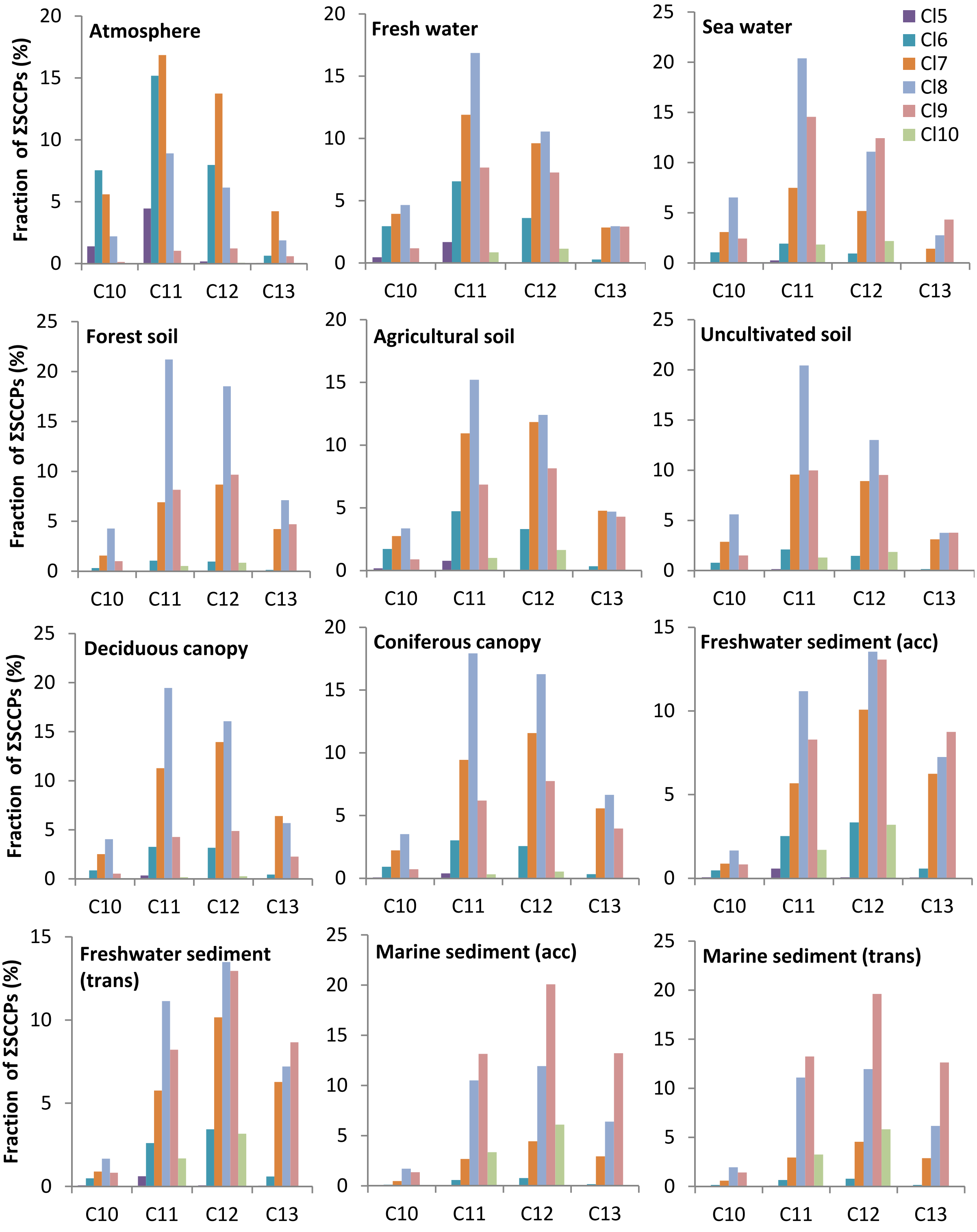

Figure S9: Predicted formula group profiles in the physical environment. Acc = accumulating, trans = transporting.

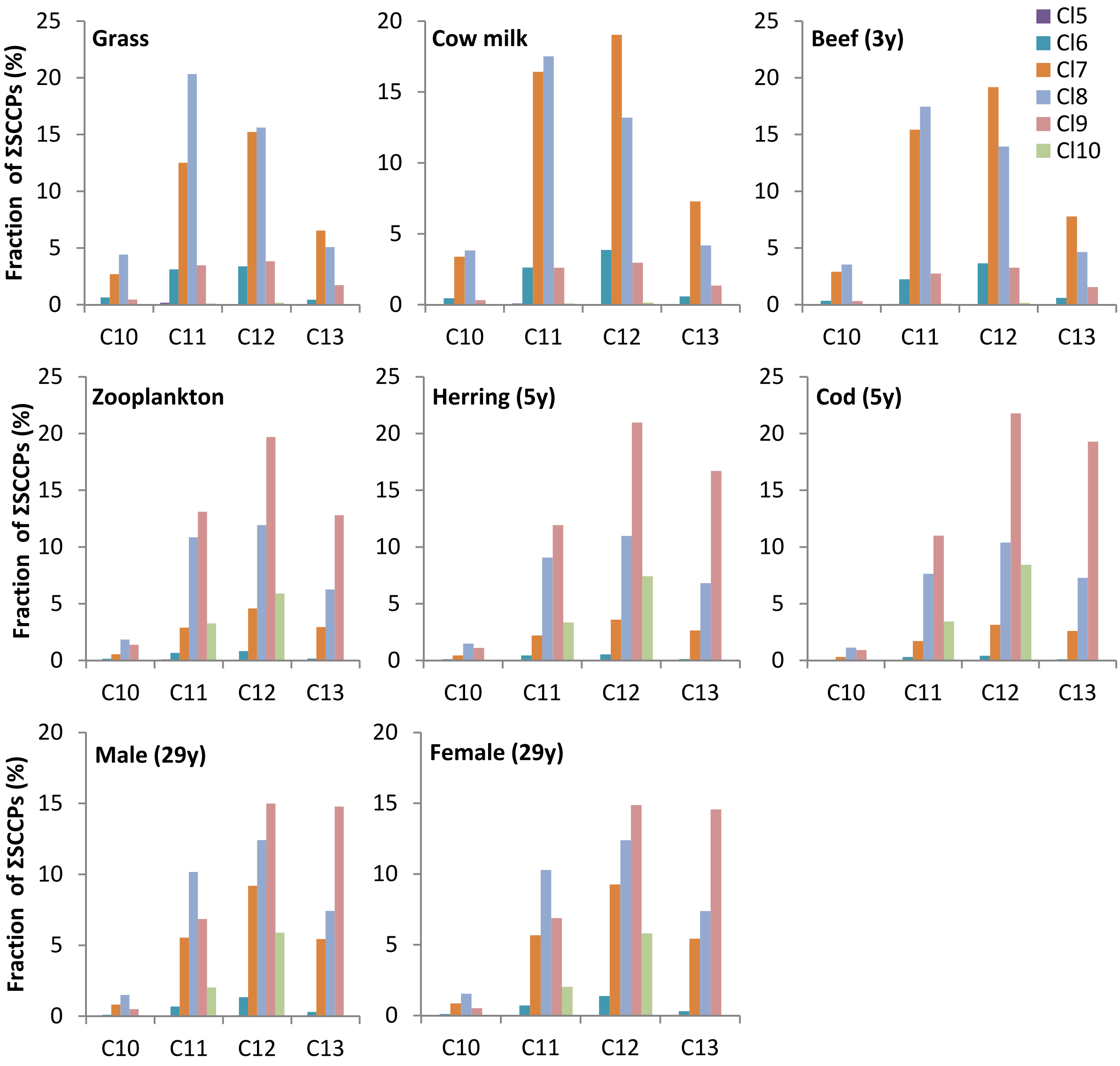

Figure S10: Predicted formula group profiles in biota. Numbers in parentheses specify the age in years of the model organism.

Figure S11: Human exposure pathways of SCCPs calculated as the fraction of total intake for a 29 year old female human deriving from air, water, or diet (dairy, beef, and fish). The exposure was calculated based on the predicted concentrations and intake rates of the various media. The predicted concentration in fish was weighted based on the age pattern of the fish and relative fractions of cod and herring in the human diet. The only difference between the exposure for males and females is that males consume 25 % more food per day, thus the fraction of SCCPs intake through air and water is reduced for males compared to females.

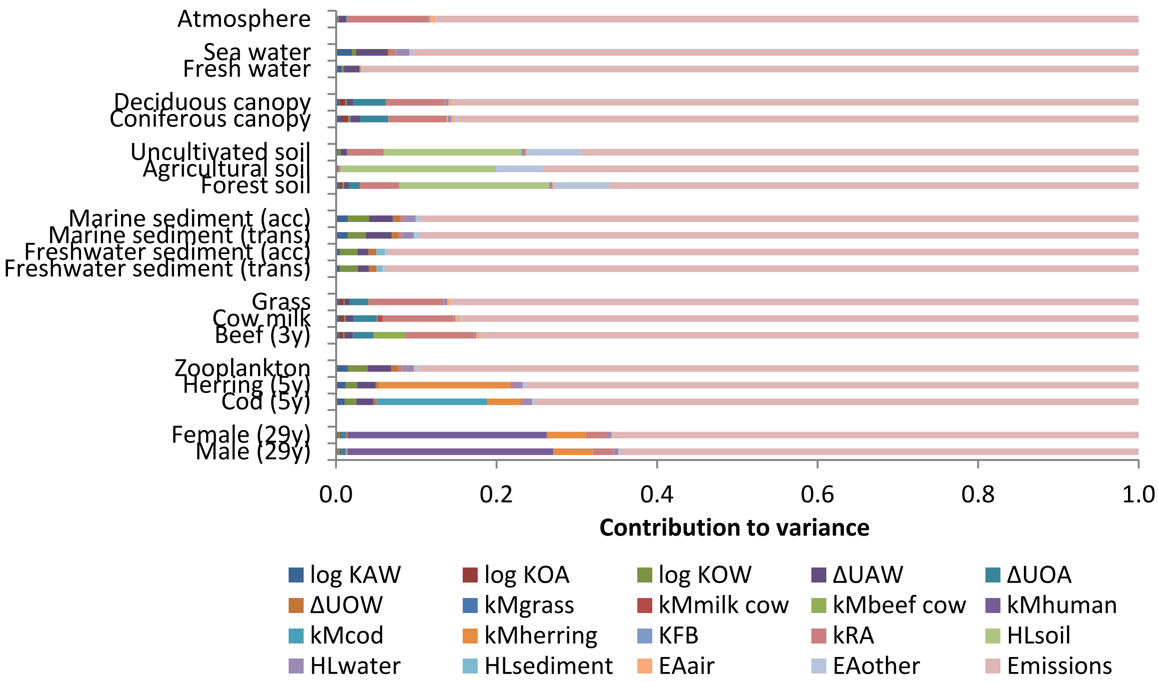

Figure S12: Contribution to variance for all physical-chemical and reactivity input parameters as well as the size of the emissions to the predicted concentration of ΣSCCPs in a given compartment, weighted by the predicted formula group distribution in the compartment. Acc = accumulating, trans = transporting, and numbers in parentheses for the biotic compartments specify the age of the model organism in years. For the size of the emissions the confidence factor (*Cf*) was set to 5 which represents the range between the predicted E_{MIN} and E_{MAX}. All sensitivities for predicted concentrations of SCCPs to the size of the emissions are 1, as the quantity of the emissions translates linearly through the model for all compartments.

3. Tables

Table S1: The number of theoretically possible SCCP isomers with a given number of carbon and chlorine atoms, and with no dichlorinated carbon atoms or branched carbon chains.[9,29] Numbers in bold are the SCCPs with 30-70 % degree of chlorination that were included in Gawor and Wania[26] and used in this study (n = 7750).

	C_{10}	C_{11}	C_{12}	C_{13}	Total
Cl_{1}	5	6	6	7	24
Cl_{2}	**25**	**30**	**36**	42	133
Cl_{3}	**60**	**85**	**110**	**146**	401
Cl_{4}	**110**	**170**	**255**	**365**	900
Cl_{5}	**126**	**236**	**396**	**651**	1409
Cl_{6}	**110**	**236**	**472**	**868**	1686
Cl_{7}	**60**	**170**	**396**	**868**	1494
Cl_{8}	**25**	**85**	**255**	**651**	1016
Cl_{9}	**5**	**30**	**110**	**365**	510
Cl_{10}	1	**6**	**36**	**146**	189
Cl_{11}	-	1	**6**	**42**	49
Cl_{12}	-	-	1	**7**	8
Cl_{13}	-	-	-	1	1
Total	527	1055	2079	4159	7820 **(7750)**

Table S2: Molecular weight (MW, g mol^{-1}), logarithmic partition coefficients (log *K*s, at 25 °C) and enthalpies of phase change (*ΔU*s, kJ mol^{-1}) for air-water ($_{AW}$), octanol-air ($_{OA}$), and octanol-water ($_{OW}$).

	MW	log K_{AW}	log K_{OA}	log K_{OW}	REF	ΔU_{AW}	ΔU_{OA}	ΔU_{OW}	REF
$C_{10} H_{20}Cl_2$	211.18	0.62	4.86	5.23	26	60.0	-80.0	-20.0	*
$C_{10} H_{19}Cl_3$	245.79	0.04	5.08	4.96	26	60.0	-80.0	-20.0	*
$C_{10} H_{18}Cl_4$	280.28	-0.61	5.48	4.78	26	60.0	-80.0	-20.0	*
$C_{10} H_{17}Cl_5$	314.77	-1.30	6.07	4.71	26	60.0	-80.0	-20.0	*
$C_{10} H_{16}Cl_6$	349.26	-2.02	6.81	4.72	26	60.0	-80.0	-20.0	*
$C_{10} H_{15}Cl_7$	383.75	-2.76	7.71	4.83	26	60.0	-80.0	-20.0	*
$C_{10}H_{14}Cl_8$	418.24	-3.51	8.72	5.03	26	60.0	-80.0	-20.0	*
$C_{10}H_{13}Cl_9$	452.73	-4.23	9.86	5.34	26	60.0	-80.0	-20.0	*
$C_{11}H_{22}Cl_2$	225.20	0.73	5.46	5.75	26	60.0	-80.0	-20.0	*
$C_{11}H_{21}Cl_3$	259.65	0.15	5.63	5.46	26	60.0	-80.0	-20.0	*
$C_{11}H_{20}Cl_4$	294.31	-0.47	5.99	5.25	26	60.0	-80.0	-20.0	*
$C_{11}H_{19}Cl_5$	328.80	-1.15	6.51	5.14	26	60.0	-80.0	-20.0	*
$C_{11}H_{18}Cl_6$	363.29	-1.86	7.18	5.11	26	60.0	-80.0	-20.0	*
$C_{11}H_{17}Cl_7$	397.78	-2.59	7.99	5.17	26	60.0	-80.0	-20.0	*
$C_{11}H_{16}Cl_8$	432.27	-3.34	8.93	5.31	26	60.0	-80.0	-20.0	*
$C_{11}H_{15}Cl_9$	466.76	-4.07	9.99	5.55	26	60.0	-80.0	-20.0	*
$C_{11}H_{14}Cl_{10}$	501.25	-4.80	11.13	5.86	26	60.0	-80.0	-20.0	*
$C_{12}H_{24}Cl_2$	239.23	0.82	6.06	6.27	26	60.0	-80.0	-20.0	*
$C_{12}H_{23}Cl_3$	273.86	0.26	6.20	5.96	26	60.0	-80.0	-20.0	*
$C_{12}H_{22}Cl_4$	308.34	-0.35	6.51	5.73	26	60.0	-80.0	-20.0	*
$C_{12}H_{21}Cl_5$	342.83	-1.01	6.97	5.59	26	60.0	-80.0	-20.0	*
$C_{12}H_{20}Cl_6$	377.32	-1.71	7.58	5.52	26	60.0	-80.0	-20.0	*
$C_{12}H_{19}Cl_7$	411.81	-2.43	8.33	5.54	26	60.0	-80.0	-20.0	*
$C_{12}H_{18}Cl_8$	446.30	-3.17	9.19	5.63	26	60.0	-80.0	-20.0	*
$C_{12}H_{17}Cl_9$	480.79	-3.91	10.17	5.81	26	60.0	-80.0	-20.0	*
$C_{12}H_{16}Cl_{10}$	515.28	-4.65	11.25	6.06	26	60.0	-80.0	-20.0	*
$C_{12}H_{15}Cl_{11}$	549.24	-5.36	12.43	6.40	26	60.0	-80.0	-20.0	*
$C_{13}H_{25}Cl_3$	287.70	0.38	6.77	6.47	26	60.0	-80.0	-20.0	*
$C_{13}H_{24}Cl_4$	322.15	-0.23	7.04	6.22	26	60.0	-80.0	-20.0	*
$C_{13}H_{23}Cl_5$	356.86	-0.87	7.46	6.05	26	60.0	-80.0	-20.0	*
$C_{13}H_{22}Cl_6$	391.35	-1.56	8.01	5.95	26	60.0	-80.0	-20.0	*
$C_{13}H_{21}Cl_7$	425.84	-2.27	8.69	5.93	26	60.0	-80.0	-20.0	*
$C_{13}H_{20}Cl_8$	460.33	-3.01	9.49	5.98	26	60.0	-80.0	-20.0	*
$C_{13}H_{19}Cl_9$	494.82	-3.75	10.41	6.10	26	60.0	-80.0	-20.0	*
$C_{13}H_{18}Cl_{10}$	529.31	-4.49	11.42	6.31	26	60.0	-80.0	-20.0	*
$C_{13}H_{17}Cl_{11}$	563.00	-5.22	12.53	6.58	26	60.0	-80.0	-20.0	*
$C_{13}H_{16}Cl_{12}$	597.71	-5.93	13.71	6.93	26	60.0	-80.0	-20.0	*
$\text{SCCP}_{\text{average}}$	386.47	-2.15	8.21	5.65	26	60.0	-80.0	-20.0	*
$\text{SCCP}_{\text{EU-RAR}}$	377.00	-2.16	8.16	6.00	27,28	60.0	-80.0	-20.0	*
PCB-28	257.54	-2.19	7.85	5.66	23	52.2	-78.5	-26.3	23
PCB-52	291.99	-2.31	8.22	5.91	23	54.1	-81.4	-27.3	23
PCB-101	326.43	-2.40	8.73	6.33	23	59.7	-83.5	-23.8	23
PCB-118	326.43	-2.67	9.36	6.69	23	60.5	-89.0	-28.5	23
PCB-138	360.88	-2.44	9.66	7.22	23	61.3	-86.3	-25.0	23
PCB-153	360.88	-2.57	9.44	6.87	23	62.8	-93.9	-31.1	23
PCB-180	395.32	-3.00	10.16	7.16	23	63.7	-92.8	-29.1	23

*Assumed values.

Table S3: Reaction rate with hydroxyl radicals (k_{RA}, cm^3 molecules^{-1} sec^{-1}, at 25 °C), environmental half-lives (hours), and activation energies (kJ mol^{-1}).

			Environmental half-lives				Activation energies		
	k_{RA}	REF	Water	Soil/Canopy	Sediment	REF	Air	Other	REF
$C_{10}H_{20}Cl_2$	7.77E-12	26	790	1580	7110	6,30,31	10.0	30.0	*
$C_{10}H_{19}Cl_3$	6.40E-12	26	1595	3189	14351	6,30,31	10.0	30.0	*
$C_{10}H_{18}Cl_4$	5.18E-12	26	3046	6092	27413	6,30,31	10.0	30.0	*
$C_{10}H_{17}Cl_5$	4.15E-12	26	5534	11068	49808	6,30,31	10.0	30.0	*
$C_{10}H_{16}Cl_6$	3.25E-12	26	9849	19698	88641	6,30,31	10.0	30.0	*
$C_{10}H_{15}Cl_7$	2.52E-12	26	17287	34573	155580	6,30,31	10.0	30.0	*
$C_{10}H_{14}Cl_8$	1.90E-12	26	29302	58605	263722	6,30,31	10.0	30.0	*
$C_{10}H_{13}Cl_9$	1.42E-12	26	45318	90637	407866	6,30,31	10.0	30.0	*
$C_{11}H_{22}Cl_2$	9.09E-12	26	785	1570	7064	6,30,31	10.0	30.0	*
$C_{11}H_{21}Cl_3$	7.62E-12	26	1598	3195	14378	6,30,31	10.0	30.0	*
$C_{11}H_{20}Cl_4$	6.34E-12	26	3089	6178	27799	6,30,31	10.0	30.0	*
$C_{11}H_{19}Cl_5$	5.19E-12	26	5708	11415	51368	6,30,31	10.0	30.0	*
$C_{11}H_{18}Cl_6$	4.20E-12	26	10268	20536	92412	6,30,31	10.0	30.0	*
$C_{11}H_{17}Cl_7$	3.34E-12	26	18221	36442	163988	6,30,31	10.0	30.0	*
$C_{11}H_{16}Cl_8$	2.62E-12	26	30764	61527	276872	6,30,31	10.0	30.0	*
$C_{11}H_{15}Cl_9$	2.02E-12	26	47223	94446	425005	6,30,31	10.0	30.0	*
$C_{11}H_{14}Cl_{10}$	1.53E-12	26	60936	121872	548426	6,30,31	10.0	30.0	*
$C_{12}H_{24}Cl_2$	1.04E-11	26	778	1557	7004	6,30,31	10.0	30.0	*
$C_{12}H_{23}Cl_3$	8.89E-12	26	1596	3192	14364	6,30,31	10.0	30.0	*
$C_{12}H_{22}Cl_4$	7.51E-12	26	3124	6247	28113	6,30,31	10.0	30.0	*
$C_{12}H_{21}Cl_5$	6.29E-12	26	5837	11673	52530	6,30,31	10.0	30.0	*
$C_{12}H_{20}Cl_6$	5.20E-12	26	10642	21283	95775	6,30,31	10.0	30.0	*
$C_{12}H_{19}Cl_7$	4.25E-12	26	19041	38083	171373	6,30,31	10.0	30.0	*
$C_{12}H_{18}Cl_8$	3.42E-12	26	32182	64365	289641	6,30,31	10.0	30.0	*
$C_{12}H_{17}Cl_9$	2.72E-12	26	49208	98415	442868	6,30,31	10.0	30.0	*
$C_{12}H_{16}Cl_{10}$	2.12E-12	26	62296	124593	560668	6,30,31	10.0	30.0	*
$C_{12}H_{15}Cl_{11}$	1.63E-12	26	74162	148324	667458	6,30,31	10.0	30.0	*
$C_{13}H_{25}Cl_3$	1.02E-11	26	1602	3203	14414	6,30,31	10.0	30.0	*
$C_{13}H_{24}Cl_4$	8.74E-12	26	3155	6310	28394	6,30,31	10.0	30.0	*
$C_{13}H_{23}Cl_5$	7.43E-12	26	5957	11913	53610	6,30,31	10.0	30.0	*
$C_{13}H_{22}Cl_6$	6.27E-12	26	10958	21917	98625	6,30,31	10.0	30.0	*
$C_{13}H_{21}Cl_7$	5.23E-12	26	19794	39589	178149	6,30,31	10.0	30.0	*
$C_{13}H_{20}Cl_8$	4.31E-12	26	33557	67114	302015	6,30,31	10.0	30.0	*
$C_{13}H_{19}Cl_9$	3.51E-12	26	50881	101762	457929	6,30,31	10.0	30.0	*
$C_{13}H_{18}Cl_{10}$	2.82E-12	26	63686	127373	573178	6,30,31	10.0	30.0	*
$C_{13}H_{17}Cl_{11}$	2.23E-12	26	74541	149081	670865	6,30,31	10.0	30.0	*
$C_{13}H_{16}Cl_{12}$	1.73E-12	26	82142	164284	739280	6,30,31	10.0	30.0	*
$SCCP_{average}$	4.85E-12	26	10916	21833	98248	6,30,31	10.0	30.0	*
$SCCP_{EU\text{-}RAR}$	3.48E-12	27,28	1.0E+11	1.0E+11	1.0E+11	27,28	10.0	30.0	*
PCB-28	1.10E-12	23	5500	10000	17000	23	10.0	30.0	23
PCB-52	5.90E-13	23	10000	17000	55000	23	10.0	30.0	23
PCB-101	3.40E-13	23	31000	100000	55000	23	10.0	30.0	23
PCB-118	3.00E-13	23	31000	100000	55000	23	10.0	30.0	23
PCB-138	1.60E-13	23	55000	170000	170000	23	10.0	30.0	23
PCB-153	1.60E-13	23	55000	550000	170000	23	10.0	30.0	23
PCB-180	1.10E-13	23	55000	1000000	170000	23	10.0	30.0	23

*Assumed values.

Table S4: Biotransformation rate constants (hour^{-1}, at 25 °C) and the feces-blood partition coefficient (K_{FB}).

	Milk cow	Beef cow	Human	Herring	Cod	REF	Grass	REF	K_{FB}	REF
$C_{10}H_{20}Cl_2$	3.94E-4	4.38E-4	7.09E-4	4.36E-3	1.87E-3	[26,*]	4.39E-4	[6,30,31]	2E-8	[32,33]
$C_{10}H_{19}Cl_3$	3.09E-4	3.43E-4	5.57E-4	3.42E-3	1.47E-3	[26,*]	2.17E-4	[6,30,31]	2E-8	[32,33]
$C_{10}H_{18}Cl_4$	2.41E-4	2.67E-4	4.33E-4	2.66E-3	1.14E-3	[26,*]	1.14E-4	[6,30,31]	2E-8	[32,33]
$C_{10}H_{17}Cl_5$	1.86E-4	2.06E-4	3.34E-4	2.05E-3	8.82E-4	[26,*]	6.26E-5	[6,30,31]	2E-8	[32,33]
$C_{10}H_{16}Cl_6$	1.43E-4	1.58E-4	2.57E-4	1.58E-3	6.77E-4	[26,*]	3.52E-5	[6,30,31]	2E-8	[32,33]
$C_{10}H_{15}Cl_7$	1.09E-4	1.21E-4	1.97E-4	1.21E-3	5.19E-4	[26,*]	2.00E-5	[6,30,31]	2E-8	[32,33]
$C_{10}H_{14}Cl_8$	8.37E-5	9.29E-5	1.51E-4	9.25E-4	3.98E-4	[26,*]	1.18E-5	[6,30,31]	2E-8	[32,33]
$C_{10}H_{13}Cl_9$	6.41E-5	7.11E-5	1.15E-4	7.09E-4	3.04E-4	[26,*]	7.65E-6	[6,30,31]	2E-8	[32,33]
$C_{11}H_{22}Cl_2$	2.84E-4	3.16E-4	5.12E-4	3.15E-3	1.35E-3	[26,*]	4.42E-4	[6,30,31]	2E-8	[32,33]
$C_{11}H_{21}Cl_3$	2.23E-4	2.48E-4	4.02E-4	2.47E-3	1.06E-3	[26,*]	2.17E-4	[6,30,31]	2E-8	[32,33]
$C_{11}H_{20}Cl_4$	1.74E-4	1.93E-4	3.13E-4	1.93E-3	8.28E-4	[26,*]	1.12E-4	[6,30,31]	2E-8	[32,33]
$C_{11}H_{19}Cl_5$	1.35E-4	1.50E-4	2.42E-4	1.49E-3	6.40E-4	[26,*]	6.07E-5	[6,30,31]	2E-8	[32,33]
$C_{11}H_{18}Cl_6$	1.04E-4	1.15E-4	1.87E-4	1.15E-3	4.93E-4	[26,*]	3.38E-5	[6,30,31]	2E-8	[32,33]
$C_{11}H_{17}Cl_7$	7.97E-5	8.84E-5	1.43E-4	8.81E-4	3.79E-4	[26,*]	1.90E-5	[6,30,31]	2E-8	[32,33]
$C_{11}H_{16}Cl_8$	6.11E-5	6.78E-5	1.10E-4	6.75E-4	2.90E-4	[26,*]	1.13E-5	[6,30,31]	2E-8	[32,33]
$C_{11}H_{15}Cl_9$	4.68E-5	5.20E-5	8.42E-5	5.18E-4	2.22E-4	[26,*]	7.34E-6	[6,30,31]	2E-8	[32,33]
$C_{11}H_{14}Cl_{10}$	3.58E-5	3.98E-5	6.45E-5	3.96E-4	1.70E-4	[26,*]	5.69E-6	[6,30,31]	2E-8	[32,33]
$C_{12}H_{24}Cl_2$	2.05E-4	2.28E-4	3.69E-4	2.27E-3	9.75E-4	[26,*]	4.45E-4	[6,30,31]	2E-8	[32,33]
$C_{12}H_{23}Cl_3$	1.61E-4	1.79E-4	2.90E-4	1.78E-3	7.67E-4	[26,*]	2.17E-4	[6,30,31]	2E-8	[32,33]
$C_{12}H_{22}Cl_4$	1.26E-4	1.40E-4	2.27E-4	1.39E-3	5.99E-4	[26,*]	1.11E-4	[6,30,31]	2E-8	[32,33]
$C_{12}H_{21}Cl_5$	9.77E-5	1.08E-4	1.76E-4	1.08E-3	4.64E-4	[26,*]	5.94E-5	[6,30,31]	2E-8	[32,33]
$C_{12}H_{20}Cl_6$	7.54E-5	8.37E-5	1.36E-4	8.34E-4	3.58E-4	[26,*]	3.26E-5	[6,30,31]	2E-8	[32,33]
$C_{12}H_{19}Cl_7$	5.80E-5	6.44E-5	1.04E-4	6.41E-4	2.76E-4	[26,*]	1.82E-5	[6,30,31]	2E-8	[32,33]
$C_{12}H_{18}Cl_8$	4.45E-5	4.94E-5	8.01E-5	4.93E-4	2.12E-4	[26,*]	1.08E-5	[6,30,31]	2E-8	[32,33]
$C_{12}H_{17}Cl_9$	3.42E-5	3.79E-5	6.15E-5	3.78E-4	1.62E-4	[26,*]	7.04E-6	[6,30,31]	2E-8	[32,33]
$C_{12}H_{16}Cl_{10}$	2.62E-5	2.91E-5	4.71E-5	2.90E-4	1.24E-4	[26,*]	5.56E-6	[6,30,31]	2E-8	[32,33]
$C_{12}H_{15}Cl_{11}$	2.01E-5	2.23E-5	3.61E-5	2.22E-4	9.54E-5	[26,*]	4.67E-6	[6,30,31]	2E-8	[32,33]
$C_{13}H_{25}Cl_3$	1.17E-4	1.29E-4	2.10E-4	1.29E-3	5.54E-4	[26,*]	2.16E-4	[6,30,31]	2E-8	[32,33]
$C_{13}H_{24}Cl_4$	9.11E-5	1.01E-4	1.64E-4	1.01E-3	4.33E-4	[26,*]	1.10E-4	[6,30,31]	2E-8	[32,33]
$C_{13}H_{23}Cl_5$	7.08E-5	7.86E-5	1.27E-4	7.83E-4	3.36E-4	[26,*]	5.82E-5	[6,30,31]	2E-8	[32,33]
$C_{13}H_{22}Cl_6$	5.47E-5	6.07E-5	9.85E-5	6.05E-4	2.60E-4	[26,*]	3.16E-5	[6,30,31]	2E-8	[32,33]
$C_{13}H_{21}Cl_7$	4.22E-5	4.68E-5	7.59E-5	4.66E-4	2.00E-4	[26,*]	1.75E-5	[6,30,31]	2E-8	[32,33]
$C_{13}H_{20}Cl_8$	3.24E-5	3.60E-5	5.83E-5	3.59E-4	1.54E-4	[26,*]	1.03E-5	[6,30,31]	2E-8	[32,33]
$C_{13}H_{19}Cl_9$	2.49E-5	2.76E-5	4.48E-5	2.75E-4	1.18E-4	[26,*]	6.81E-6	[6,30,31]	2E-8	[32,33]
$C_{13}H_{18}Cl_{10}$	1.91E-5	2.12E-5	3.44E-5	2.11E-4	9.08E-5	[26,*]	5.44E-6	[6,30,31]	2E-8	[32,33]
$C_{13}H_{17}Cl_{11}$	1.47E-5	1.63E-5	2.64E-5	1.62E-4	6.97E-5	[26,*]	4.65E-6	[6,30,31]	2E-8	[32,33]
$C_{13}H_{16}Cl_{12}$	1.12E-5	1.25E-5	2.02E-5	1.24E-4	5.34E-5	[26,*]	4.22E-6	[6,30,31]	2E-8	[32,33]
SCCP$_{average}$	7.58E-5	8.42E-5	1.36E-4	8.39E-4	3.60E-4	[26,*]	3.17E-5	[6,30,31]	2E-8	[32,33]
SCCP$_{EU\text{-}RAR}$	7.58E-5	8.42E-5	1.36E-4	8.39E-4	3.60E-4	[26,*]	6.93E-12	[27,28]	2E-8	[32,33]
PCB-28	9.32E-3	9.32E-3	5.48E-5	0	0	[23]	0	[23]	2E-8	[23]
PCB-52	9.32E-3	9.32E-3	7.42E-4	0	0	[23]	0	[23]	2E-8	[23]
PCB-101	9.32E-3	9.32E-3	2.28E-4	0	0	[23]	0	[23]	2E-8	[23]
PCB-118	0	0	1.26E-5	0	0	[23]	0	[23]	2E-8	[23]
PCB-138	0	0	9.13E-6	0	0	[23]	0	[23]	2E-8	[23]
PCB-153	0	0	5.25E-6	0	0	[23]	0	[23]	2E-8	[23]
PCB-180	0	0	3.42E-7	0	0	[23]	0	[23]	2E-8	[23]

* Adjusted to geometric mean of body-weight according to Arnot et al.[34,35]

Table S5: Formula group composition of analytical standards (Qstd) and commercial mixtures (Cmix) used for estimating the formula group composition of the emissions. Qstd marked with * is an average based on routine analysis in our own laboratory, and the number in parenthesis indicate the number of standards that the average is calculated from. The specified chlorination degree (%Cl) is as indicated from the manufacturer, while the calculated %Cl is estimated from the formula group composition and the %Cl of the individual formula groups. It should be noted that the numbers for the formula group composition are approximate, as many of them are based on approximate readings from figures in the referenced papers. Values below 0.01 have not been included in the table (-), but were counted as zero in the calculation of the averages.

Reference	Qstd *(2)	Qstd *(13)	Qstd[14]	Qstd[12]	Qstd[15]	Qstd[12]	Qstd[13]	Qstd[11]	Qstd[10]	**Average**	**Average**	Cmix[9]	Cmix[16]	Qstd *(2)	Cmix[9]	**Average**	**FINAL**
Specified %Cl	51.0	55.5	55.5	55.5	55.5	55.5	55.5	55.5	55.5	**55.5**	**50-59**	60	60	63.0	70	**60-70**	
Calculated %Cl	59.2	60.7	60.4	61.8	60.7	60.8	59.4	60.7	59.5	**60.5**	**59.8**	60.8	61.9	64.0	65.4	**63.0**	**61.4**
C_{10} $H_{17}Cl_5$	1.6	1.3	1.1	0.3	1.0	-	1.0	0.3	1.0	0.7	1.1	1.7	1.4	0.04	-	0.8	**0.9**
C_{10} $H_{16}Cl_6$	4.6	4.1	2.6	3.9	4.4	2.6	2.0	2.6	2.9	3.0	3.8	11.7	8.2	2.8	1.4	6.0	**4.9**
C_{10} $H_{15}Cl_7$	3.4	4.0	1.5	1.9	3.4	1.9	1.3	2.1	2.0	2.0	2.7	4.7	6.6	3.6	3.4	4.6	**3.6**
$C_{10}H_{14}Cl_8$	0.07	0.3	0.3	1.0	2.5	1.9	1.0	2.4	1.0	1.4	0.8	1.1	2.7	2.6	6.1	3.1	**1.9**
$C_{10}H_{13}Cl_9$	-	0.03	-	0.3	-	0.3	-	0.8	-	0.2	0.1	0.3	0.3	0.4	1.4	0.6	**0.3**
$C_{11}H_{19}Cl_5$	9.6	5.8	2.1	0.6	2.0	1.0	3.3	1.3	2.9	1.9	5.8	5.0	2.2	0.1	-	1.8	**3.8**
$C_{11}H_{18}Cl_6$	18.0	13.0	11.2	9.1	16.7	11.7	12.4	10.6	16.7	12.6	15.3	21.2	12.8	2.9	0.7	9.4	**12.4**
$C_{11}H_{17}Cl_7$	9.2	15.5	14.7	21.4	17.2	14.9	11.4	14.3	13.7	15.4	12.3	16.2	22.1	10.3	12.9	15.4	**13.8**
$C_{11}H_{16}Cl_8$	1.7	3.9	3.7	7.8	4.9	5.8	3.6	5.8	2.9	4.9	3.3	7.8	8.7	18.9	25.5	15.2	**9.3**
$C_{11}H_{15}Cl_9$	0.05	0.3	0.4	1.3	1.0	1.0	0.7	0.8	1.0	0.9	0.5	0.8	1.9	4.6	12.9	5.1	**2.8**
$C_{11}H_{14}Cl_{10}$	-	0.02	-	0.3	-	-	-	0.3	-	0.08	0.0	-	0.3	0.8	1.7	0.7	**0.4**
$C_{12}H_{21}Cl_5$	-	-	-	-	-	-	2.3	1.1	2.0	0.8	0.4	-	-	-	-	-	**0.2**
$C_{12}H_{20}Cl_6$	15.5	10.0	11.9	4.5	11.8	9.7	12.1	9.8	14.7	10.6	13.0	6.7	4.9	0.4	-	3.0	**8.0**
$C_{12}H_{19}Cl_7$	18.8	19.2	19.3	19.4	17.2	18.8	16.3	18.8	16.7	18.1	18.5	13.1	14.2	8.4	4.1	9.9	**14.2**
$C_{12}H_{18}Cl_8$	3.0	5.4	8.8	10.4	5.9	7.5	5.9	6.9	3.9	7.0	5.0	6.7	7.9	16.0	12.2	10.7	**7.9**
$C_{12}H_{17}Cl_9$	0.3	0.9	1.2	2.6	1.0	1.6	1.0	1.6	1.0	1.4	0.9	0.6	2.5	9.6	12.2	6.2	**3.5**
$C_{12}H_{16}Cl_{10}$	0.01	0.04	0.1	0.3	-	-	-	0.3	-	0.1	0.1	-	0.5	1.8	2.4	1.2	**0.6**
$C_{13}H_{23}Cl_5$	-	-	-	-	-	-	1.3	-	1.0	0.3	0.2	-	-	-	-	-	**0.1**
$C_{13}H_{22}Cl_6$	-	-	-	-	-	4.2	6.8	5.0	5.9	3.1	1.6	-	-	-	-	-	**0.8**
$C_{13}H_{21}Cl_7$	11.1	2.4	11.9	4.5	6.9	8.4	11.1	8.5	6.9	8.3	9.7	1.4	1.1	2.4	-	1.2	**5.5**
$C_{13}H_{20}Cl_8$	2.6	5.0	7.6	7.8	3.0	6.5	5.5	5.3	2.9	5.5	4.1	0.6	1.1	5.1	1.4	2.0	**3.0**
$C_{13}H_{19}Cl_9$	0.5	8.9	1.7	2.6	1.0	1.9	1.3	1.6	1.0	1.6	1.1	0.3	0.5	9.1	1.7	2.9	**2.0**

Table S6: Absolute sensitivities, as average ± standard deviation of all SCCP$_{37}$ formula groups, for model results to partition coefficients (*K*s) and enthalpies of phase change (*ΔU*s). The model results include the characteristic travel distance (L_A), mass remaining in the environment 10 years after emission stop (M_{10Y}), and concentrations in the specified compartments after 70 years of emissions. Sed (acc) = accumulating sediment, sed (trans) = transporting sediment, and numbers in parentheses for the biotic compartments specify the age of the model organism in years. Only absolute average sensitivities of 0.01 or higher have been included, and average sensitivities of 0.20 or higher are highlighted in bold.

	K_{AW}	K_{OA}	K_{OW}	ΔU_{AW}	ΔU_{OA}	ΔU_{OW}
L_A	0.14 ± 0.24	0.07 ± 0.15	0.05 ± 0.09	**0.33 ± 0.49**	**0.20 ± 0.43**	0.03 ± 0.05
M_{10Y}	0.02 ± 0.02	0.02 ± 0.02	0.15 ± 0.17	0.02 ± 0.02	0.04 ± 0.03	0.11 ± 0.13
Male (29y)	**0.24 ± 0.22**	**0.22 ± 0.29**	**0.38 ± 0.33**	**0.20 ± 0.20**	**0.49 ± 0.68**	0.08 ± 0.08
Female (29y)	**0.22 ± 0.20**	**0.21 ± 0.29**	**0.35 ± 0.31**	0.19 ± 0.18	**0.48 ± 0.67**	0.08 ± 0.08
Cod (5y)	**0.30 ± 0.29**	0.01 ± 0.01	**0.58 ± 0.25**	**0.47 ± 0.43**	0.03 ± 0.03	**0.31 ± 0.15**
Herring (5y)	**0.30 ± 0.29**	0.01 ± 0.02	**0.58 ± 0.25**	**0.47 ± 0.44**	0.03 ± 0.03	**0.32 ± 0.15**
Zooplankton	**0.30 ± 0.28**	0.01 ± 0.01	**0.76 ± 0.33**	**0.47 ± 0.43**	0.03 ± 0.03	**0.45 ± 0.20**
Beef (3y)	**0.40 ± 0.28**	**0.50 ± 0.42**	**0.28 ± 0.27**	**0.50 ± 0.33**	**1.12 ± 0.98**	0.15 ± 0.09
Cow milk	**0.34 ± 0.24**	**0.45 ± 0.42**	**0.21 ± 0.18**	**0.45 ± 0.33**	**1.00 ± 0.97**	0.15 ± 0.11
Grass	**0.24 ± 0.23**	**0.58 ± 0.42**	0.10 ± 0.14	**0.39 ± 0.27**	**1.51 ± 1.27**	0.07 ± 0.08
Freshwater sed (trans)	0.12 ± 0.14		**0.57 ± 0.26**	**0.21 ± 0.25**		**0.40 ± 0.21**
Freshwater sed (acc)	0.12 ± 0.15		**0.57 ± 0.26**	**0.20 ± 0.25**		**0.40 ± 0.21**
Marine sed (trans)	**0.29 ± 0.29**	0.01 ± 0.01	**0.71 ± 0.31**	**0.51 ± 0.44**	0.03 ± 0.03	**0.43 ± 0.19**
Marine sed (acc)	**0.30 ± 0.29**	0.01 ± 0.01	**0.80 ± 0.35**	**0.49 ± 0.44**	0.03 ± 0.03	**0.48 ± 0.22**
Forest soil	**0.20 ± 0.15**	**0.33 ± 0.17**	0.17 ± 0.13	**0.30 ± 0.22**	**0.81 ± 0.49**	0.10 ± 0.08
Agricultural soil	0.07 ± 0.05	0.01 ± 0.01	0.07 ± 0.04	0.12 ± **0.07**	0.02 ± 0.02	0.04 ± 0.03
Uncultivated soil	**0.38 ± 0.27**	0.03 ± 0.02	**0.39 ± 0.23**	**0.82 ± 0.63**	0.10 ± **0.06**	**0.27 ± 0.19**
Coniferous canopy	0.19 ± 0.22	**0.43 ± 0.22**	0.12 ± 0.14	**0.29 ± 0.30**	**1.12 ± 0.72**	0.07 ± 0.08
Deciduous canopy	0.19 ± 0.21	**0.45 ± 0.28**	0.12 ± 0.14	**0.29 ± 0.26**	**1.31 ± 0.95**	0.07 ± 0.08
Fresh water	0.13 ± 0.16		**0.21 ± 0.13**	**0.22 ± 0.26**		0.15 ± 0.07
Sea water	**0.30 ± 0.29**	0.01 ± 0.01	0.19 ± 0.26	**0.47 ± 0.43**	0.03 ± 0.03	0.11 ± 0.15
Air	**0.24 ± 0.28**	0.09 ± 0.14	0.12 ± 0.13	**0.46 ± 0.50**	**0.24 ± 0.39**	0.07 ± 0.07

Table S7: Absolute sensitivities, as average ± standard deviation of all SCCP$_{37}$ formula groups, for model results to the atmospheric degradation rate (k_{RA}), environmental half-lives, and activation energies. The model results include the characteristic travel distance (L_A), mass remaining in the environment 10 years after emission stop (M_{10Y}), and concentrations in the specified compartments after 70 years of emissions. Acc = accumulating, trans = transporting, and numbers in parentheses for the biotic compartments specify the age of the model organism in years. Only absolute average sensitivities of 0.01 or higher have been included, and average sensitivities of 0.20 or higher are highlighted in bold.

	k_{RA}	Half-lives			Activation energies	
		Soil	Water	Sediment	Air	Other
L_A	**0.79 ± 0.34**		0.01 ± 0.02		**0.28 ± 0.14**	0.01 ± 0.02
M_{10Y}	0.06 ± 0.04	**0.22 ± 0.19**	0.01 ± 0.02	**0.67 ± 1.02**	0.02 ± 0.01	**0.77 ± 0.84**
Male (29y)	**0.35 ± 0.31**	0.01 ± 0.01	0.10 ± 0.08	0.02 ± 0.01	0.10 ± 0.08	0.10 ± 0.06
Female (29y)	**0.35 ± 0.31**	0.01 ± 0.01	0.10 ± 0.08	0.01 ± 0.01	0.10 ± 0.09	0.10 ± 0.06
Cod (5y)	0.12 ± 0.13		0.11 ± 0.09	0.01 ± 0.01	0.04 ± 0.04	0.10 ± 0.07
Herring (5y)	0.13 ± 0.13		0.11 ± 0.08	0.01 ± 0.02	0.04 ± 0.04	0.10 ± 0.07
Zooplankton	0.12 ± 0.13		0.11 ± 0.09	0.01 ± 0.01	0.04 ± 0.04	0.10 ± 0.07
Beef (3y)	**0.64 ± 0.32**	0.02 ± 0.01	0.06 ± 0.05	0.01 ± 0.01	0.17 ± 0.09	0.07 ± 0.04
Cow milk	**0.59 ± 0.33**	0.01 ± 0.01	0.07 ± 0.06	0.01 ± 0.01	0.16 ± 0.10	0.08 ± 0.05
Grass	**0.74 ± 0.31**	0.01 ± 0.01	0.07 ± 0.06	0.01 ± 0.01	**0.23 ± 0.13**	0.08 ± 0.06
Freshwater sed (trans)	0.01 ± 0.02		0.03 ± 0.04	**0.31 ± 0.25**		**0.33 ± 0.27**
Freshwater sed (acc)	0.01 ± 0.02		0.04 ± 0.04	**0.35 ± 0.27**		**0.35 ± 0.28**
Marine sed (trans)	0.12 ± 0.13	0.01 ± 0.01	0.11 ± 0.08	**0.23 ± 0.22**	0.03 ± 0.04	**0.30 ± 0.21**
Marine sed (acc)	0.13 ± 0.13		0.11 ± 0.08	**0.16 ± 0.17**	0.04 ± 0.04	**0.24 ± 0.17**
Forest soil	**0.67 ± 0.30**	**0.76 ± 0.15**	0.06 ± 0.06	0.01 ± 0.01	0.19 ± 0.11	**0.72 ± 0.14**
Agricultural soil	0.07 ± 0.06	**0.75 ± 0.14**	0.01 ± 0.02		0.02 ± 0.02	**0.65 ± 0.12**
Uncultivated soil	**0.67 ± 0.34**	**0.75 ± 0.15**	0.06 ± 0.05	0.01 ± 0.01	**0.22 ± 0.13**	**0.71 ± 0.14**
Coniferous canopy	**0.69 ± 0.31**	0.05 ± 0.03	0.06 ± 0.06	0.01 ± 0.01	**0.21 ± 0.12**	0.11 ± 0.06
Deciduous canopy	**0.68 ± 0.31**	0.02 ± 0.01	0.07 ± 0.06	0.01 ± 0.01	**0.22 ± 0.12**	0.08 ± 0.05
Fresh water	0.01 ± 0.02		0.04 ± 0.04	0.02 ± 0.02		0.06 ± 0.04
Sea water	0.13 ± 0.13		0.11 ± 0.08	0.01 ± 0.01	0.04 ± 0.04	0.10 ± 0.07
Air	**0.69 ± 0.33**	0.01 ± 0.01	0.07 ± 0.06	0.01 ± 0.01	**0.21 ± 0.12**	0.07 ± 0.05

Table S8: Absolute sensitivities, as average ± standard deviation of all SCCP$_{37}$ formula groups, for model results to biotransformation rate constants and the feces-blood partition coefficient (K_{FB}). The model results include concentrations in biota after 70 years of emissions, and numbers in parentheses specify the age of the model organism in years. Only absolute average sensitivities of 0.01 or higher have been included, and average sensitivities of 0.20 or higher are highlighted in bold.

	Biotransformation rate constants						K_{FB}
	Grass	Milk cattle	Beef cattle	Human	Cod	Herring	
Male (29y)	0.01 ± 0.01	0.04 ± 0.04	0.03 ± 0.03	**0.80 ± 0.19**	0.02 ± 0.01	**0.37 ± 0.23**	0.03 ± 0.02
Female (29y)		0.04 ± 0.04	0.03 ± 0.03	**0.79 ± 0.17**	0.01 ± 0.01	**0.36 ± 0.23**	0.02 ± 0.02
Cod (5y)					**0.73 ± 0.16**	**0.28 ± 0.11**	
Herring (5y)						**0.73 ± 0.13**	
Zooplankton							
Beef (3y)	0.01 ± 0.01		**0.33 ± 0.14**				
Cow milk	0.01 ± 0.01	0.13 ± 0.06					
Grass	0.01 ± 0.01						

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