

Electronic Supplementary Information (ESI)

The influence of chemical degradation during dietary exposures to fish on biomagnification factors and bioaccumulation factors

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ESI – 1: Bioaccumulation endpoint definitions

The bioaccumulation factor (BAF; L/kg) is a field measurement defined as the steady state ratio of the chemical concentration in an aquatic organism, i.e. fish, to the chemical concentration in the exposure water ^{1, 2}. The BAF is normalized to the exposure water; however, the BAF includes exposure pathways from the surrounding water and from the diet. The biomagnification factor (BMF; kg/kg) can be measured in the environment and is defined as the steady state ratio of the chemical concentration in a predator to the chemical concentration in its prey ^{1, 2}. The BMF can also be measured in the laboratory using steady state concentration ratios or kinetically using rate constants, i.e., $BMF_K = k_D/k_T$, where k_D is the dietary uptake rate constant (kg/kg/h) and k_T is the total elimination rate constant (/h) ³. The BMF measured in the environment includes exposures from the diet (including in some cases ingested sediment) and water and the laboratory BMF includes exposures from the diet only. In both exposure scenarios the BMF is normalized to dietary exposure and for neutral organic chemicals it is preferable to measure and report the BMF on a lipid weight basis to assess biomagnification potential in terms of chemical thermodynamics ⁴.

ESI – 2: Existing E_D - K_{OW} regression models

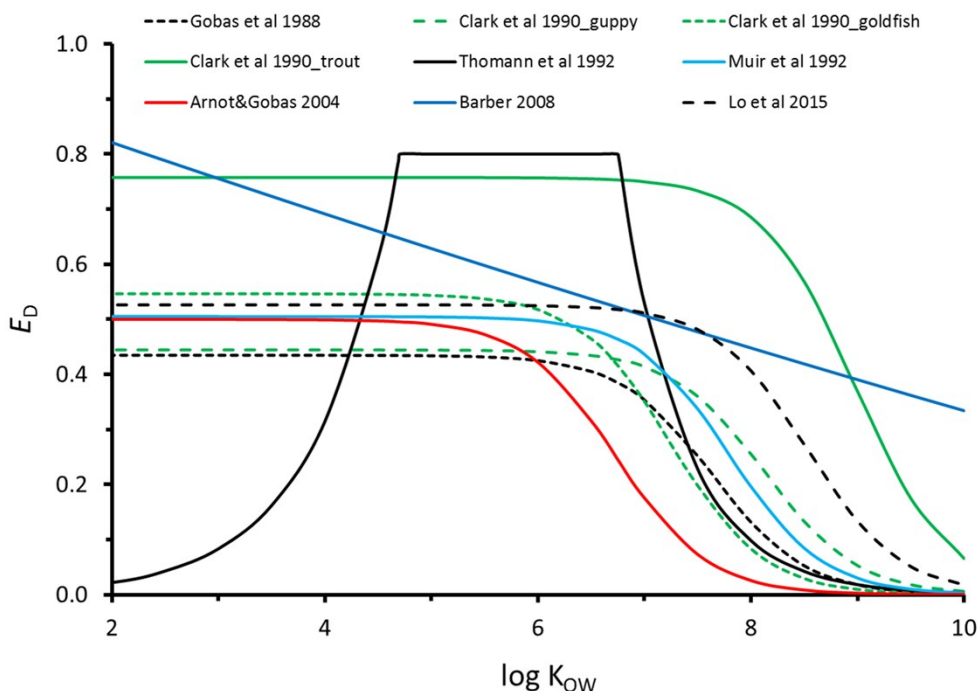


Figure ESI-1. Summary of existing E_D - K_{OW} regression models as a function of K_{OW} .

ESI – 3: Empirical E_D data compilation and selection

Forty years of fish dietary bioaccumulation testing data have been collected and critically reviewed ⁵ including 1,199 measurements for E_D determined from various experimental methods. Variation in dietary testing methods ⁵ has been significant. For example, dietary exposure durations range from a single bolus dose (<1 d) to 286 d (median=20) ⁵. Dietary matrices range from natural food to various commercial food pellets with measured lipid contents ranging from 0.2% to 24% (median=14%) and feeding rates range from 0.4% to 12.4% body weight per day (median=2%) ⁵. Test design variability and other factors propagate variability in measured E_D (and F) and resulting in different E_D - K_{OW} regressions dependent on the empirical data selected for the regression (e.g., Figure 2, Figure ESI-1). We applied the following selection criteria to partially address the variability in the E_D data:

- Following the data quality review criteria described by Arnot and Quinn ⁵, only E_D values that were scored as high (H) or medium (M) data confidence were selected;
- Fish were exposed to chemical daily for at least 8 days;
- Fish were fed at a consistent rate, i.e., % body weight, and at consistent exposure levels;
- Tests using radiolabelled chemicals were not considered;
- Tests with ionizable organics were not considered;
- Only chemicals with evidence of negligible or very slow biotransformation in fish were selected ⁶.

ESI – 4: Model calibration

Table ESI-1 summarizes the model calibration dataset. Figure ESI-2 is plot of the residuals between model predictions and observations.

Table ESI-1: Summary of the E_D model calibration dataset

Chemical name	Log Kow	Species	Measured E_D	Ref.	Modelled E_D
1,2,4,5,6,7,8,8-Octachloro-2,3,3a,4,7,7a-Hexahydro-4,7-methano-1H-indene	6.22	Rainbow trout	0.55	7	0.50
1,2,4,5,6,7,8,8-Octachloro-2,3,3a,4,7,7a-Hexahydro-4,7-methano-1H-indene	6.22	Rainbow trout	0.65	7	0.50
1,2,4,5,6,7,8,8-Octachloro-2,3,3a,4,7,7a-Hexahydro-4,7-methano-1H-indene	6.22	Rainbow trout	0.60	7	0.50
1,2,4,5-Tetrachlorobenzene	4.64	Goldfish	0.50	8	0.51
1,2,4,5-Tetrachlorobenzene	4.64	Goldfish	0.46	8	0.51
1,2,4,5-Tetrachlorobenzene	4.64	Goldfish	0.50	8	0.51
1,2,4,5-Tetrachlorobenzene	4.64	Goldfish	0.74	9	0.51
1,2,4,5-Tetrachlorobenzene	4.64	Rainbow trout	0.63	10	0.51
2,2',3,3',4,4',5,5',6-Nonachlorobiphenyl	8.09	Rainbow trout	0.53	11	0.34
2,2',3,3',4,4',5,5',6-Nonachlorobiphenyl	8.09	Rainbow trout	0.44	11	0.34
2,2',3,3',4,4',5,5'-Octachlorobiphenyl	7.80	Guppy	0.40	12	0.41
2,2',3,3',4,4',5,5'-Octachlorobiphenyl	7.80	Guppy	0.31	12	0.41
2,2',3,3',4,4',5,5'-Octachlorobiphenyl	7.80	Goldfish	0.35	8	0.41
2,2',3,3',4,4',5,5'-Octachlorobiphenyl	7.80	Goldfish	0.53	8	0.41
2,2',3,3',4,4',5,5'-Octachlorobiphenyl	7.80	Goldfish	0.48	8	0.41
2,2',3,3',4,4',5,6'-Octachlorobiphenyl	7.65	Guppy	0.24	13	0.43
2,2',3,3',4,4',5,6'-Octachlorobiphenyl	7.65	Guppy	0.18	13	0.43
2,2',3,3',4,4',5,6'-Octachlorobiphenyl	7.65	Guppy	0.12	13	0.43
2,2',3,3',4,4',5,6'-Octachlorobiphenyl	7.65	Guppy	0.35	13	0.43
2,2',3,3',4,4',5,6'-Octachlorobiphenyl	7.65	Guppy	0.27	13	0.43
2,2',3,3',4,4',5,6'-Octachlorobiphenyl	7.65	Guppy	0.59	13	0.43
2,2',3,3',4,4',5,6-Octachlorobiphenyl	7.56	Rainbow trout	0.49	11	0.44
2,2',3,3',4,4',6-Heptachlorobiphenyl	7.11	Rainbow trout	0.49	11	0.48
2,2',3,3',4,5,5',6,6'-Nonachlorobiphenyl	7.71	Rainbow trout	0.48	11	0.42
2,2',3,3',4,5',6,6'-Octachlorobiphenyl	7.62	Rainbow trout	0.49	11	0.44
2,2',3,3',4,5,6'-Heptachlorobiphenyl	7.11	Rainbow trout	0.54	14	0.48
2,2',3,3',4,5',6-Heptachlorobiphenyl	7.15	Rainbow trout	0.52	11	0.48
2,2',3,3',4,5'-Hexachlorobiphenyl	6.80	Marbled sole	0.41	15	0.49
2,2',3,3',4,5-Hexachlorobiphenyl	6.94	Rainbow trout	0.57	11	0.49
2,2',3,3',4,6,6'-Heptachlorobiphenyl	6.78	Rainbow trout	0.51	11	0.49

Chemical name	Log Kow	Species	Measured E_D	Ref.	Modelled E_D
2,2',3,3',4,6'-Hexachlorobiphenyl	6.58	Rainbow trout	0.58	11	0.50
2,2',3,3',4,6'-Hexachlorobiphenyl	6.58	Rainbow trout	0.47	11	0.50
2,2',3,3',4-Pentachlorobiphenyl	6.20	Marbled sole	0.37	15	0.50
2,2',3,3',5,5',6,6'-Octachlorobiphenyl	7.13	Rainbow trout	0.51	11	0.48
2,2',3,3',5,5',6,6'-Octachlorobiphenyl	7.13	Rainbow trout	0.44	11	0.48
2,2',3,3',5,6'-Hexachlorobiphenyl	6.64	Marbled sole	0.32	15	0.50
2,2',3,3',5-Pentachlorobiphenyl	6.26	Marbled sole	0.34	15	0.50
2,2',3,3',6,6'-Hexachlorobiphenyl	6.22	Rainbow trout	0.54	11	0.50
2,2',3,3',6,6'-Hexachlorobiphenyl	6.22	Rainbow trout	0.45	11	0.50
2,2',3,3',6,6'-Hexachlorobiphenyl	6.22	Rainbow trout	0.54	7	0.50
2,2',3,3',6,6'-Hexachlorobiphenyl	6.22	Rainbow trout	0.50	7	0.50
2,2',3,3',6,6'-Hexachlorobiphenyl	6.22	Rainbow trout	0.52	7	0.50
2,2',3,3'-Tetrachlorobiphenyl	5.66	Rainbow trout	0.49	11	0.51
2,2',3,3'-Tetrachlorobiphenyl	5.66	Marbled sole	0.30	15	0.51
2,2',3,4,4',5,6'-Heptachlorobiphenyl	7.20	Rainbow trout	0.48	11	0.48
2,2',3,4,4',5',6-Heptachlorobiphenyl	7.20	Marbled sole	0.44	15	0.48
2,2',3,4,4',5'-Hexachlorobiphenyl	6.83	Rainbow trout	0.49	16	0.49
2,2',3,4',5,5',6-Heptachlorobiphenyl	7.17	Rainbow trout	0.45	16	0.48
2,2',3,4',5',6-Hexachlorobiphenyl	6.67	Marbled sole	0.40	15	0.50
2,2',3,4',6'-Pentachlorobiphenyl	6.13	Marbled sole	0.34	15	0.50
2,2',3,4'-Tetrachlorobiphenyl	5.76	Rainbow trout	0.54	11	0.50
2,2',3,4'-Tetrachlorobiphenyl	5.76	Rainbow trout	0.50	11	0.50
2,2',3,4'-Tetrachlorobiphenyl	5.76	Marbled sole	0.37	15	0.50
2,2',3,4-Tetrachlorobiphenyl	5.69	Rainbow trout	0.53	11	0.50
2,2',3,4-Tetrachlorobiphenyl	5.69	Rainbow trout	0.48	11	0.50
2,2',3,5,5'-Pentachlorobiphenyl	6.35	Rainbow trout	0.56	11	0.50
2,2',3,5,5'-Pentachlorobiphenyl	6.35	Rainbow trout	0.49	11	0.50
2,2',3,5',6-Pentachlorobiphenyl	6.13	Rainbow trout	0.80	7	0.50
2,2',3,5',6-Pentachlorobiphenyl	6.13	Rainbow trout	0.80	7	0.50
2,2',3,5',6-Pentachlorobiphenyl	6.13	Rainbow trout	0.81	7	0.50
2,2',3,5'-Tetrachlorobiphenyl	5.75	Rainbow trout	0.54	11	0.50
2,2',3,5'-Tetrachlorobiphenyl	5.75	Rainbow trout	0.49	11	0.50
2,2',3,5'-Tetrachlorobiphenyl	5.75	Rainbow trout	0.34	16	0.50
2,2',3,5'-Tetrachlorobiphenyl	5.75	Rainbow trout	0.42	16	0.50
2,2',3,5'-Tetrachlorobiphenyl	5.75	Marbled sole	0.36	15	0.50

Chemical name	Log Kow	Species	Measured E_D	Ref.	Modelled E_D
2,2',3,5-Tetrachlorobiphenyl	5.76	Rainbow trout	0.53	11	0.50
2,2',3,5-Tetrachlorobiphenyl	5.76	Rainbow trout	0.50	11	0.50
2,2',3,6'-Tetrachlorobiphenyl	5.53	Rainbow trout	0.47	11	0.51
2,2',3,6'-Tetrachlorobiphenyl	5.53	Marbled sole	0.28	15	0.51
2,2',3,6-Tetrachlorobiphenyl	5.53	Rainbow trout	0.56	11	0.51
2,2',3,6-Tetrachlorobiphenyl	5.53	Marbled sole	0.24	15	0.51
2,2',3-Trichlorobiphenyl	5.16	Rainbow trout	0.56	11	0.51
2,2',3-Trichlorobiphenyl	5.16	Rainbow trout	0.46	11	0.51
2,2',3-Trichlorobiphenyl	5.16	Marbled sole	0.31	15	0.51
2,2',4,4',5,5'-Hexachlorobiphenyl	6.92	Guppy	0.61	12	0.49
2,2',4,4',5,5'-Hexachlorobiphenyl	6.92	Guppy	0.51	12	0.49
2,2',4,4',5,5'-Hexachlorobiphenyl	6.92	Rainbow trout	0.46	10	0.49
2,2',4,4'-Tetrachlorobiphenyl	5.85	Rainbow trout	0.54	11	0.50
2,2',4,4'-Tetrachlorobiphenyl	5.85	Rainbow trout	0.49	11	0.50
2,2',4,6'-Tetrachlorobiphenyl	5.63	Rainbow trout	0.50	11	0.51
2,2',4,6'-Tetrachlorobiphenyl	5.63	Rainbow trout	0.49	11	0.51
2,2',4,6'-Tetrachlorobiphenyl	5.63	Marbled sole	0.37	15	0.51
2,2',4-Trichlorobiphenyl	5.25	Marbled sole	0.34	15	0.51
2,2',5,5'-Tetrachlorobiphenyl	5.84	Guppy	0.42	12	0.50
2,2',5,5'-Tetrachlorobiphenyl	5.84	Guppy	0.51	12	0.50
2,2',5,5'-Tetrachlorobiphenyl	5.84	Rainbow trout	0.49	11	0.50
2,2',5,5'-Tetrachlorobiphenyl	5.84	Guppy	0.83	13	0.50
2,2',5,5'-Tetrachlorobiphenyl	5.84	Goldfish	0.44	8	0.50
2,2',5,5'-Tetrachlorobiphenyl	5.84	Goldfish	0.47	8	0.50
2,2',5,5'-Tetrachlorobiphenyl	5.84	Goldfish	0.47	8	0.50
2,2',5,5'-Tetrachlorobiphenyl	5.84	Goldfish	0.69	9	0.50
2,2',5,5'-Tetrachlorobiphenyl	5.84	Guppy	0.75	9	0.50
2,2',5,5'-Tetrachlorobiphenyl	5.84	Rainbow trout	0.45	10	0.50
2,2',5,6'-Tetrachlorobiphenyl	5.62	Marbled sole	0.27	15	0.51
2,2',5-Trichlorobiphenyl	5.24	Rainbow trout	0.50	11	0.51
2,2',5-Trichlorobiphenyl	5.24	Rainbow trout	0.51	11	0.51
2,2',5-Trichlorobiphenyl	5.24	Rainbow trout	0.31	16	0.51
2,2',5-Trichlorobiphenyl	5.24	Rainbow trout	0.32	16	0.51
2,2',5-Trichlorobiphenyl	5.24	Marbled sole	0.28	15	0.51
2,2',6,6'-Tetrachlorobiphenyl	5.40	Rainbow trout	0.56	11	0.51

Chemical name	Log Kow	Species	Measured E_D	Ref.	Modelled E_D
2,2',6-Trichlorobiphenyl	5.02	Rainbow trout	0.56	11	0.51
2,2'-Dichlorophenyl	4.65	Rainbow trout	0.61	11	0.51
2,3,3',4'-Tetrachlorobiphenyl	6.11	Rainbow trout	0.49	11	0.50
2,3,3',4'-Tetrachlorobiphenyl	6.11	Rainbow trout	0.42	11	0.50
2,3,3',6-Tetrachlorobiphenyl	5.95	Rainbow trout	0.50	11	0.50
2,3,3',6-Tetrachlorobiphenyl	5.95	Rainbow trout	0.49	11	0.50
2,3,3'-Trichlorobiphenyl	5.57	Marbled sole	0.25	15	0.51
2,3',4,4',5,5'-Hexachlorobiphenyl	7.27	Rainbow trout	0.55	11	0.47
2,3',4,4',5-Pentachlorobiphenyl	6.74	Rainbow trout	0.55	16	0.50
2,3',4',5,5'-Pentachlorobiphenyl	6.73	Marbled sole	0.51	15	0.50
2,3,4',5-Tetrachlorobiphenyl	6.17	Rainbow trout	0.48	11	0.50
2,3',4',5'-Tetrachlorobiphenyl	6.13	Rainbow trout	0.56	11	0.50
2,3,4',6-Tetrachlorobiphenyl	5.95	Rainbow trout	0.55	11	0.50
2,3,4',6-Tetrachlorobiphenyl	5.95	Rainbow trout	0.52	11	0.50
2,3',4',6-Tetrachlorobiphenyl	5.98	Marbled sole	0.39	15	0.50
2,3,4'-Trichlorobiphenyl	5.58	Rainbow trout	0.51	11	0.51
2,3,4'-Trichlorobiphenyl	5.58	Rainbow trout	0.48	11	0.51
2,3',4'-Trichlorobiphenyl	5.60	Rainbow trout	0.53	11	0.51
2,3',4'-Trichlorobiphenyl	5.60	Rainbow trout	0.47	11	0.51
2,3',4'-Trichlorobiphenyl	5.67	Rainbow trout	0.48	11	0.50
2,3',5-Trichlorobiphenyl	5.66	Rainbow trout	0.50	11	0.51
2,3',5-Trichlorobiphenyl	5.66	Rainbow trout	0.49	11	0.51
2,3,6-Trichlorobiphenyl	5.40	Rainbow trout	0.53	11	0.51
2,3,6-Trichlorobiphenyl	5.40	Rainbow trout	0.43	11	0.51
2,3',6-Trichlorobiphenyl	5.44	Marbled sole	0.33	15	0.51
2,3'-Dichlorobiphenyl	5.06	Rainbow trout	0.45	11	0.51
2,3'-Dichlorobiphenyl	5.06	Rainbow trout	0.43	11	0.51
2,4,4',5-Tetrachlorobiphenyl	6.20	Rainbow trout	0.52	11	0.50
2,4,4'-Trichlorobiphenyl	5.67	Rainbow trout	0.39	16	0.50
2,4,4'-Trichlorobiphenyl	5.67	Rainbow trout	0.45	16	0.50
2,4',5-Trichlorobiphenyl	5.67	Rainbow trout	0.52	11	0.50
2,4',5-Trichlorobiphenyl	5.67	Rainbow trout	0.50	11	0.50
2,4,6,2',4',6'-Hexachlorobiphenyl	7.18	Guppy	0.74	13	0.48
2,4,6,2',4',6'-Hexachlorobiphenyl	7.18	Goldfish	0.33	8	0.48
2,4,6,2',4',6'-Hexachlorobiphenyl	7.18	Goldfish	0.42	8	0.48

Chemical name	Log Kow	Species	Measured E_D	Ref.	Modelled E_D
2,4,6,2',4',6'-Hexachlorobiphenyl	7.18	Goldfish	0.36	8	0.48
2,4,6,2',4',6'-Hexachlorobiphenyl	7.18	Goldfish	0.69	9	0.48
2,4,6,2',4',6'-Hexachlorobiphenyl	7.18	Guppy	0.65	9	0.48
2,4,6,2',4',6'-Hexachlorobiphenyl	7.18	Rainbow trout	0.46	10	0.48
2,4',6-Trichlorobiphenyl	5.44	Rainbow trout	0.50	11	0.51
2,4',6-Trichlorobiphenyl	5.44	Rainbow trout	0.48	11	0.51
2,4',6-Trichlorobiphenyl	5.44	Marbled sole	0.34	15	0.51
2,4'-Dichlorobiphenyl	5.07	Rainbow trout	0.46	11	0.51
2,4'-Dichlorobiphenyl	5.07	Rainbow trout	0.45	11	0.51
2,4'-Dichlorobiphenyl	5.07	Marbled sole	0.21	15	0.51
3,3',4,4',5-Pentachlorobiphenyl	6.89	Rainbow trout	0.54	17	0.49
3,3',4,4',5-Pentachlorobiphenyl	6.89	Rainbow trout	0.68	17	0.49
3,3',4,4',5-Pentachlorobiphenyl	6.89	Rainbow trout	0.62	17	0.49
3,4-Dichlorobiphenyl	5.22	Rainbow trout	0.58	11	0.51
4,4'-Dibromobiphenyl	5.72	Guppy	0.65	13	0.50
4,4'-Dichlorobiphenyl	5.28	Rainbow trout	0.50	11	0.51
4,4'-Dichlorobiphenyl	5.28	Rainbow trout	0.48	11	0.51
Decachlorobiphenyl	8.18	Guppy	0.26	12	0.32
Decachlorobiphenyl	8.18	Guppy	0.19	12	0.32
Decachlorobiphenyl	8.18	Rainbow trout	0.40	11	0.32
Decachlorobiphenyl	8.18	Goldfish	0.26	8	0.32
Decachlorobiphenyl	8.18	Goldfish	0.34	8	0.32
Decachlorobiphenyl	8.18	Goldfish	0.30	8	0.32
Decachlorobiphenyl	8.18	Rainbow trout	0.34	10	0.32
Hexachlorobenzene	5.73	Guppy	0.20	13	0.50
Hexachlorobenzene	5.73	Guppy	0.55	13	0.50
Hexachlorobenzene	5.73	Guppy	0.17	13	0.50
Hexachlorobenzene	5.73	Guppy	0.22	13	0.50
Hexachlorobenzene	5.73	Guppy	0.24	13	0.50
Hexachlorobenzene	5.73	Rainbow trout	0.55	5	0.50
Hexachlorobenzene	5.73	Rainbow trout	0.43	5	0.50
Hexachlorobenzene	5.73	Rainbow trout	0.54	5	0.50
Hexachlorobenzene	5.73	Rainbow trout	0.68	5	0.50
Hexachlorobenzene	5.73	Rainbow trout	0.57	5	0.50
Hexachlorobenzene	5.73	Rainbow trout	0.35	5	0.50

Chemical name	Log Kow	Species	Measured E_D	Ref.	Modelled E_D
Hexachlorobenzene	5.73	Rainbow trout	0.42	5	0.50
Hexachlorobenzene	5.73	Rainbow trout	0.18	5	0.50
Hexachlorobenzene	5.73	Rainbow trout	0.34	16	0.50
Hexachlorobenzene	5.73	Rainbow trout	0.50	16	0.50
Hexachlorobenzene	5.73	Goldfish	0.46	8	0.50
Hexachlorobenzene	5.73	Goldfish	0.50	8	0.50
Hexachlorobenzene	5.73	Goldfish	0.46	8	0.50
Hexachlorobenzene	5.73	Goldfish	0.71	9	0.50
Hexachlorobenzene	5.73	Guppy	0.57	9	0.50
Hexachlorobenzene	5.73	Common carp	0.49	18	0.50
Hexachlorobenzene	5.73	Common carp	0.76	18	0.50
Hexachlorobenzene	5.73	Common carp	0.78	18	0.50
Hexachlorobenzene	5.73	Common carp	0.86	18	0.50
Hexachlorobenzene	5.73	Common carp	0.73	18	0.50
Hexachlorobenzene	5.73	Common carp	0.75	18	0.50
Hexachlorobenzene	5.73	Common carp	0.72	19	0.50
Hexachlorobenzene	5.73	Common carp	0.73	19	0.50
Hexachlorobenzene	5.73	Rainbow trout	0.53	10	0.50
Hexachlorobenzene	5.73	Rainbow trout	0.47	20	0.50
Hexachlorobenzene	5.73	Rainbow trout	0.50	20	0.50
Hexachlorobenzene	5.73	Rainbow trout	0.74	20	0.50
Hexachlorobenzene	5.73	Rainbow trout	0.79	20	0.50
Hexachlorobenzene	5.73	Common carp	0.39	20	0.50
Hexachlorobenzene	5.73	Common carp	0.41	20	0.50
Hexachlorobenzene	5.73	Common carp	0.38	20	0.50
Hexachlorobenzene	5.73	Common carp	0.40	20	0.50
Hexachlorobenzene	5.73	Common carp	0.31	20	0.50
Hexachlorobenzene	5.73	Common carp	0.33	20	0.50
Hexachlorobenzene	5.73	Rainbow trout	0.51	20	0.50
Hexachlorobenzene	5.73	Rainbow trout	0.54	20	0.50
Hexachlorobenzene	5.73	Rainbow trout	0.67	20	0.50
Hexachlorobenzene	5.73	Rainbow trout	0.70	20	0.50
Hexachlorobenzene	5.73	Rainbow trout	0.73	20	0.50
Hexachlorobenzene	5.73	Rainbow trout	0.77	20	0.50
Hexachlorobenzene	5.73	Rainbow trout	0.30	20	0.50

Chemical name	Log Kow	Species	Measured E_D	Ref.	Modelled E_D
Hexachlorobenzene	5.73	Rainbow trout	0.32	20.	0.50
Hexachlorobenzene	5.73	Rainbow trout	0.57	20.	0.50
Hexachlorobenzene	5.73	Rainbow trout	0.60	20.	0.50
Hexachlorobenzene	5.73	Rainbow trout	0.74	20.	0.50
Hexachlorobenzene	5.73	Rainbow trout	0.67	20.	0.50
Hexachlorobenzene	5.73	Rainbow trout	0.60	20.	0.50
Hexachlorobenzene	5.73	Rainbow trout	0.89	20.	0.50
Hexachlorobenzene	5.73	Rainbow trout	0.67	20.	0.50
Hexachlorobenzene	5.73	Rainbow trout	0.25	20.	0.50
Hexachlorobenzene	5.73	Rainbow trout	0.74	20.	0.50
Hexachlorobenzene	5.73	Catfish	0.67	21	0.50
Mirex	6.89	Guppy	0.21	13	0.49
Mirex	6.89	Guppy	0.16	13	0.49
Mirex	6.89	Guppy	0.27	13	0.49
Mirex	6.89	Guppy	0.24	13	0.49
Mirex	6.89	Goldfish	0.51	9	0.49
Mirex	6.89	Guppy	0.56	9	0.49
Musk-xylene	4.45	Common carp	0.54	18	0.51
Musk-xylene	4.45	Rainbow trout	0.35	20.	0.51
Musk-xylene	4.45	Rainbow trout	0.42	20.	0.51
Musk-xylene	4.45	Rainbow trout	0.95	20.	0.51
Musk-xylene	4.45	Common carp	0.54	20.	0.51
Musk-xylene	4.45	Common carp	0.48	20.	0.51
Musk-xylene	4.45	Common carp	0.31	20.	0.51
Musk-xylene	4.45	Rainbow trout	0.66	20.	0.51
Musk-xylene	4.45	Rainbow trout	0.36	20.	0.51
Musk-xylene	4.45	Rainbow trout	0.43	20.	0.51
Musk-xylene	4.45	Rainbow trout	0.24	20.	0.51
Musk-xylene	4.45	Rainbow trout	0.58	20.	0.51
Musk-xylene	4.45	Rainbow trout	0.58	20.	0.51
Musk-xylene	4.45	Rainbow trout	0.78	20.	0.51
Musk-xylene	4.45	Rainbow trout	0.66	20.	0.51
Musk-xylene	4.45	Rainbow trout	0.66	20.	0.51
Musk-xylene	4.45	Rainbow trout	0.15	20.	0.51
Musk-xylene	4.45	Rainbow trout	0.73	20.	0.51

Chemical name

Octachlorostyrene
 Octachlorostyrene
 Octachlorostyrene
 p,p'-DDD
 Pentachlorobenzene
 Pentachlorobenzene
 Pentachlorobenzene
 Pentachlorobenzene
 Pentachlorobenzene
 Pentachlorobenzene

Log Kow	Species	Measured E_D	Ref.	Modelled E_D
7.46	Goldfish	0.48	8	0.46
7.46	Goldfish	0.66	8	0.46
7.46	Goldfish	0.62	8	0.46
6.02	Rainbow trout	0.67	14	0.50
5.17	Goldfish	0.46	8	0.51
5.17	Goldfish	0.48	8	0.51
5.17	Goldfish	0.51	8	0.51
5.17	Goldfish	0.51	9	0.51
5.17	Guppy	0.55	9	0.51
5.17	Rainbow trout	0.55	10	0.51

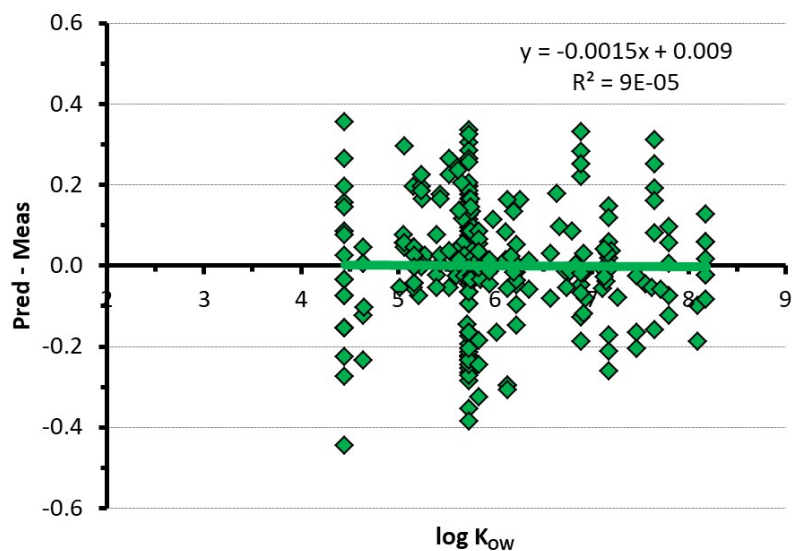


Figure ESI-2. Plot of residuals for model calibration dataset.

ESI – 5: New k_R database

Table ESI-2 summarizes the new k_R estimates obtained with the evaluated E_D database and the new E_D model.

Table ESI-2: Summary of the new k_R estimates.

Chemical name	Log Kow	Species	Measured E_D	Ref.	Modelled E_D	Estimated k_R /d
(1 alpha,2 alpha,3 beta,4 alpha,5 beta,6 beta)1,2,3,4,5,6-Hexachlorocyclohexane	3.80	Rainbow trout	0.07	14	0.50	1.06E+01
(1 alpha,2 alpha,3 beta,4 alpha,5 beta,6 beta)1,2,3,4,5,6-Hexachlorocyclohexane	3.80	Rainbow trout	0.45	22	0.50	2.08E-01
(1 alpha,2 alpha,3 beta,4 alpha,5 beta,6 beta)1,2,3,4,5,6-Hexachlorocyclohexane	3.80	Rainbow trout	0.09	7	0.50	7.94E+00
(1 alpha,2 alpha,3 beta,4 alpha,5 beta,6 beta)1,2,3,4,5,6-Hexachlorocyclohexane	3.80	Rainbow trout	0.09	7	0.50	8.16E+00
(1 alpha,2 alpha,3 beta,4 alpha,5 beta,6 beta)1,2,3,4,5,6-Hexachlorocyclohexane	3.80	Rainbow trout	0.08	7	0.50	8.51E+00
(1 alpha,2 alpha,3 beta,4 alpha,5 beta,6 beta)1,2,3,4,5,6-Hexachlorocyclohexane	3.80	Rainbow trout	0.05	7	0.50	1.71E+01
(1 alpha,2 alpha,3 beta,4 alpha,5 beta,6 beta)1,2,3,4,5,6-Hexachlorocyclohexane	3.80	Rainbow trout	0.04	7	0.50	1.79E+01
(1 alpha,2 alpha,3 beta,4 alpha,5 beta,6 beta)1,2,3,4,5,6-Hexachlorocyclohexane	3.80	Rainbow trout	0.04	7	0.50	1.84E+01
1,1'-(2,2,2-Trichloroethylidene)bis[4-methoxy-benzene	5.08	Common carp	0.16	23	0.51	3.58E+00
1,1'-(2,2,2-Trichloroethylidene)bis[4-methoxy-benzene	5.08	Rainbow trout	0.13	20	0.51	4.87E+00
1,1'-(2,2,2-Trichloroethylidene)bis[4-methoxy-benzene	5.08	Rainbow trout	0.34	20	0.51	8.34E-01
1,1'-(2,2,2-Trichloroethylidene)bis[4-methoxy-benzene	5.08	Rainbow trout	0.28	20	0.51	1.37E+00
1,1'-(2,2,2-Trichloroethylidene)bis[4-methoxy-benzene	5.08	Rainbow trout	0.24	20	0.51	1.88E+00
1,1'-(2,2,2-Trichloroethylidene)bis[4-methoxy-benzene	5.08	Rainbow trout	0.23	20	0.51	2.03E+00

Chemical name	Log Kow	Species	Measured E_D	Ref.	Modelled E_D	Estimated k_R /d
1,1'-(2,2,2-Trichloroethylidene)bis[4-methoxy-benzene	5.08	Rainbow trout	0.21	20	0.51	2.39E+00
1,1'-(2,2,2-Trichloroethylidene)bis[4-methoxy-benzene	5.08	Rainbow trout	0.14	20	0.51	4.40E+00
1,1'-(2,2,2-Trichloroethylidene)bis[4-methoxy-benzene	5.08	Rainbow trout	0.14	20	0.51	4.40E+00
1,1'-(2,2,2-Trichloroethylidene)bis[4-methoxy-benzene	5.08	Rainbow trout	0.13	20	0.51	4.87E+00
1,1'-(2,2,2-Trichloroethylidene)bis[4-methoxy-benzene	5.08	Common carp	0.13	20	0.51	4.87E+00
1,1'-(2,2,2-Trichloroethylidene)bis[4-methoxy-benzene	5.08	Rainbow trout	0.12	20	0.51	5.41E+00
1,1'-(2,2,2-Trichloroethylidene)bis[4-methoxy-benzene	5.08	Rainbow trout	0.11	20	0.51	6.05E+00
1,1'-(2,2,2-Trichloroethylidene)bis[4-methoxy-benzene	5.08	Common carp	0.10	20	0.51	6.82E+00
1,1'-(2,2,2-Trichloroethylidene)bis[4-methoxy-benzene	5.08	Rainbow trout	0.06	20	0.51	1.25E+01
1,1'-(2,2,2-Trichloroethylidene)bis[4-methoxy-benzene	5.08	Common carp	0.06	20	0.51	1.25E+01
1,1,3,3,5-Pentamethylindan (liquid)	6.30	Rainbow trout	0.23	24	0.50	2.00E+00
1,1':3',1''Tercyclohexane	8.55	Rainbow trout	0.12	5	0.21	1.02E+00
1,2,13,14-Tetrachlorotetradecane	8.09	Rainbow trout	0.33	25	0.34	5.09E-02
1,2,3,10b-Tetrahydrofluoranthene	4.39	Rainbow trout	0.30	24	0.51	1.17E+00
1,2,3,4 Tetramethyl benzene	4.00	Rainbow trout	0.44	10	0.50	2.54E-01
1,2,3,4 Tetramethylbenzene	4.00	Rainbow trout	0.20	24	0.50	2.58E+00
1,2,3,4,4a,7,8,9,10,11,12,12a-dodecahydrochrysene	6.94	Rainbow trout	0.18	5	0.49	2.87E+00
1,2,3,4,5,6,7,8-octahydrophenanthrene	5.92	Rainbow trout	0.19	5	0.50	2.80E+00
1,2,3,4,5,6-Hexahydrochrysene	6.07	Rainbow trout	0.49	5	0.50	4.83E-02
1,2,3,4,7,8-Hexachlorodibenzofuran	7.92	Zebrafish	0.20	26	0.38	1.39E+00
1,2,3,4,7,8-Hexachlorodibenzo-p-dioxin	7.80	Zebrafish	0.30	26	0.41	5.53E-01
1,2,3,4-Tetrahydro-1,4-Dimethyl naphthalene (1,4-Dimethyl Tetralin)	4.79	Rainbow trout	0.40	24	0.51	4.55E-01
1,2,3,6,7,8 Hexahydropyrene	6.12	Rainbow trout	0.17	5	0.50	3.31E+00
1,2,5,6,9,10-Hexachlorodecane	6.48	Rainbow trout	0.46	25	0.50	1.50E-01
1,2,9,10-Tetrachlorodecane	6.12	Rainbow trout	0.23	25	0.50	2.01E+00
1,3,5-Tribromobenzene	4.51	Guppy	0.27	13	0.51	1.49E+00

Chemical name	Log Kow	Species	Measured E_D	Ref.	Modelled E_D	Estimated k_R/d
1,3,5-Trimethylbenzene	3.66	Rainbow trout	0.04	24	0.50	1.94E+01
1,3,5-Trimethylcyclohexane	4.43	Rainbow trout	0.23	24	0.51	2.03E+00
1,3-Dimethyladamantane	4.84	Rainbow trout	0.10	24	0.51	6.82E+00
1-decene	5.70	Rainbow trout	0.50	5	0.50	1.72E-02
1-decene	5.70	Rainbow trout	0.07	24	0.50	1.04E+01
1-dodecene	6.10	Rainbow trout	0.29	5	0.50	1.25E+00
1-dodecene	6.10	Rainbow trout	0.11	24	0.50	6.01E+00
1-ethylpyrene	5.97	Rainbow trout	0.09	24	0.50	7.72E+00
1H-1,2,4-Triazole, 1-[2-(2,4-Dichlorophenyl)pentyl]-	4.67	Rainbow trout	0.09	14	0.51	7.52E+00
1-Heptadecyne	7.92	Rainbow trout	0.22	5	0.38	1.12E+00
1-Hexadecene	8.06	Rainbow trout	0.30	24	0.35	2.44E-01
1-methyl-7-(1methylethyl)-hydrophenanthrene	6.96	Rainbow trout	0.13	24	0.49	4.58E+00
1-methyl-7-(1methylethyl)-phenanthrene	6.35	Rainbow trout	0.50	24	0.50	5.53E-03
1-Methylphenanthrene	5.08	Rainbow trout	0.02	24	0.51	3.86E+01
1-octylpyrene	8.92	Rainbow trout	0.03	24	0.12	3.71E+00
1-tert butyl-4-methyl benzene	5.17	Rainbow trout	0.40	24	0.51	4.55E-01
1-Tridecene	6.59	Rainbow trout	0.20	24	0.50	2.51E+00
1-undecene	5.61	Rainbow trout	0.30	24	0.51	1.17E+00
2 - Isopropyl Decalin	5.52	Rainbow trout	0.03	5	0.51	2.65E+01
2 - Isopropyl Decalin	5.52	Rainbow trout	0.03	5	0.51	3.09E+01
2 - Isopropyl Decalin	5.52	Rainbow trout	0.19	24	0.51	2.81E+00
2,2',3,4,4',5',6-Heptabromodiphenyl ether	7.49	Lake trout	0.35	27	0.45	4.72E-01
2,2',3,4,4',5',6-Heptabromodiphenyl ether	7.49	Zebrafish	0.09	28	0.45	6.10E+00
2,2',3,4,4',5',6-Heptabromodiphenyl ether	7.49	Zebrafish	0.09	28	0.45	6.35E+00
2,2',3,4,4',5'-Hexabromodiphenyl ether	7.09	Lake trout	0.25	27	0.48	1.55E+00
2,2',3,4,4'-Pentabromodiphenyl ether	6.69	Lake trout	0.20	27	0.50	2.49E+00
2,2,3-Trimethyl decane	6.54	Rainbow trout	0.17	5	0.50	3.25E+00
2,2,3-Trimethyl decane	6.54	Rainbow trout	0.04	5	0.50	2.21E+01
2,2',4,4',5,5'-Hexabromodiphenyl ether	7.09	Lake trout	0.40	27	0.48	3.49E-01
2,2',4,4',5,6-Hexabromodiphenyl ether	7.09	Lake trout	0.40	27	0.48	3.49E-01
2,2',4,4',5-Pentabromodiphenyl ether	6.69	Lake trout	0.45	27	0.50	1.78E-01
2,2,4,4,6,6 pentamethyl-3-heptene	5.85	Rainbow trout	0.09	24	0.50	7.74E+00
2,2,4,4,6,8,8-heptamethylnonane	7.79	Rainbow trout	0.03	24	0.41	1.94E+01

Chemical name	Log Kow	Species	Measured E_D	Ref.	Modelled E_D	Estimated k_R/d
2,2',4,4',6-Pentabromodiphenyl ether	6.69	Lake trout	0.45	27	0.50	1.78E-01
2,2',4,4'-Tetrabromodiphenyl ether	6.29	Lake trout	0.45	27	0.50	2.00E-01
2,2,4,6,6-pentamethylheptane	5.94	Rainbow trout	0.07	5	0.50	1.04E+01
2,2,4,6,6-pentamethylheptane	5.94	Rainbow trout	0.07	24	0.50	1.04E+01
2,2,5,7-Tetramethyltetraline	5.92	Rainbow trout	0.18	24	0.50	3.04E+00
2,3,3',4,4',5,6-Heptabromodiphenyl ether	7.49	Lake trout	0.35	27	0.45	4.72E-01
2,3,4,4'-Tetrabromodiphenyl ether	6.29	Lake trout	0.20	27	0.50	2.55E+00
2,3,6,7-Tetramethylanthracene	6.53	Rainbow trout	0.03	24	0.50	2.61E+01
2,3-Dimethy-5(4methylpentyl) naphthalene	7.19	Rainbow trout	0.30	5	0.48	9.83E-01
2,3-Dimethy-5(4methylpentyl) naphthalene	7.19	Rainbow trout	0.30	24	0.48	9.83E-01
2,3-Dimethyldecane	6.09	Rainbow trout	0.16	5	0.50	3.62E+00
2,3-Dimethyldecane	6.09	Rainbow trout	0.02	5	0.50	5.09E+01
2,3-Dimethylheptane	4.61	Rainbow trout	0.17	5	0.51	3.25E+00
2,3-Dimethylheptane	4.61	Rainbow trout	0.17	24	0.51	3.34E+00
2,3-Dimethylnaphthalene	4.40	Rainbow trout	0.12	24	0.51	5.41E+00
2,4,4'-Tribromodiphenyl ether	5.88	Lake trout	0.45	27	0.50	2.09E-01
2,4,4'-Tribromodiphenyl ether	5.88	sole	0.16	29	0.50	3.60E+00
2,4,6-Tribromobiphenyl	4.13	Guppy	0.32	13	0.51	9.88E-01
2,4,6-Tribromophenol	4.13	Zebrafish	0.45	28	0.51	2.12E-01
2,4,6-Trimethyl-3-heptene	4.95	Rainbow trout	0.14	24	0.51	4.40E+00
2,4-Dichloro-1-(4-nitrophenoxy) benzene	4.64	Common carp	0.50	23	0.51	3.01E-02
2,4-Dichloro-1-(4-nitrophenoxy) benzene	4.64	Common carp	0.38	19	0.51	5.68E-01
2,4-Dichloro-1-(4-nitrophenoxy) benzene	4.64	Common carp	0.41	19	0.51	4.23E-01
2,6,10-Trimethyl dodecane	7.49	Rainbow trout	0.18	5	0.45	2.43E+00
2,6-Dimethyldecane	6.09	Rainbow trout	0.31	5	0.50	1.06E+00
2,6-Dimethyldecane	6.09	Rainbow trout	0.03	24	0.50	2.31E+01
2,6-Dimethyldecane	6.09	Rainbow trout	0.33	10	0.50	8.98E-01
2,6-Dimethyloctane	5.11	Rainbow trout	0.04	5	0.51	1.85E+01
2,6-Dimethylundecane	6.58	Rainbow trout	0.09	5	0.50	7.69E+00
2,7-Di-isopropyl decalin	6.85	Rainbow trout	0.07	24	0.49	1.00E+01
2,7-Diisopropyl naphthalene	6.08	Rainbow trout	0.04	5	0.50	1.94E+01
2,7-Diisopropyl naphthalene	6.08	Rainbow trout	0.40	24	0.50	4.45E-01
2-butyl-1-decene	7.14	Rainbow trout	0.12	24	0.48	4.94E+00
2-hexyl Tetralin	6.96	Rainbow trout	0.03	5	0.49	2.52E+01
2-methyl-1-dodecene	6.65	Rainbow trout	0.12	24	0.50	5.26E+00

Chemical name	Log Kow	Species	Measured E_D	Ref.	Modelled E_D	Estimated k_R/d
2-methyl-1-nonene	5.17	Rainbow trout	0.20	24	0.51	2.59E+00
2-methyl-1-tridecene	7.14	Rainbow trout	0.19	5	0.48	2.53E+00
2-methyl-1-undecene	6.15	Rainbow trout	0.20	24	0.50	2.56E+00
2-methyldecane	5.67	Rainbow trout	0.30	24	0.50	1.17E+00
2-Methylnaphthalene	3.86	Rainbow trout	0.10	24	0.50	6.79E+00
2-methylundecane	6.16	Rainbow trout	0.07	5	0.50	9.87E+00
3,3',4,4' Tetramethyl 1,1'-biphenyl	5.95	Rainbow trout	0.08	5	0.50	8.90E+00
3,3',4,4'-Tetrabromodiphenyl ether	6.29	Lake trout	0.40	27	0.50	4.39E-01
3,3',5,5' Tetramethylbibenzyl	6.93	Rainbow trout	0.25	5	0.49	1.61E+00
3,5,5-Trimethylcyclohexene	4.25	Rainbow trout	0.30	24	0.51	1.17E+00
3,5,5'-Trimethylhexene	4.44	Rainbow trout	0.20	24	0.51	2.59E+00
3-ethyl-nonane	5.67	Rainbow trout	0.10	5	0.50	6.81E+00
3-methyl-1-hexylcyclohexane	6.47	Rainbow trout	0.07	5	0.50	1.04E+01
3-methylcholanthrene	6.42	Rainbow trout	0.50	24	0.50	2.92E-03
3-methyldecane	5.67	Rainbow trout	0.06	5	0.50	1.37E+01
3-Phenyl bicyclohexyl	7.50	Rainbow trout	0.29	5	0.45	8.99E-01
4,5,9,10-Tetrahydropyrene	5.04	Rainbow trout	0.16	24	0.51	3.65E+00
4-ethyl-1,1'-biphenyl	4.80	Rainbow trout	0.03	5	0.51	2.66E+01
4-ethyl-1,1'-biphenyl	4.80	Rainbow trout	0.50	24	0.51	1.96E-02
4-methyl dodecane	6.65	Rainbow trout	0.08	5	0.50	8.57E+00
5-ethyl-1-nonene	5.53	Rainbow trout	0.38	5	0.51	5.66E-01
5-ethyl-1-nonene	5.53	Rainbow trout	0.29	5	0.51	1.27E+00
5 α (H)-androsterane	6.65	Rainbow trout	0.14	5	0.50	4.27E+00
6-ethylchrysene	6.56	Rainbow trout	0.15	24	0.50	3.90E+00
6-methylchrysene	6.07	Rainbow trout	0.30	24	0.50	1.16E+00
6-n-Butyl-2,3-Dimethylnaphthalene	6.28	Rainbow trout	0.03	24	0.50	2.63E+01
7-Methylbenz(a)anthracene	6.07	Rainbow trout	0.05	5	0.50	1.52E+01
7-Methylbenz(a)anthracene	6.07	Rainbow trout	0.20	24	0.50	2.57E+00
9-Methyl anthracene	5.07	Rainbow trout	0.13	10	0.51	4.87E+00
9-n butylphenanthrene	6.37	Rainbow trout	0.04	24	0.50	1.93E+01
Anthracene	4.45	Rainbow trout	0.10	5	0.51	6.82E+00
Anthracene	4.45	Rainbow trout	0.30	24	0.51	1.17E+00
Anthracene	4.45	Rainbow trout	0.02	24	0.51	4.06E+01
anti-Decchlorane Plus	9.00	Rainbow trout	0.04	30	0.10	2.02E+00

Chemical name	Log Kow	Species	Measured E_D	Ref.	Modelled E_D	Estimated k_R /d
Benzene, 1,1'-(1,1,2,2-tetramethyl-1,2-ethaneDiyl)bis-	6.48	Rainbow trout	0.18	5	0.50	2.99E+00
Benzene, 1,3,5-Tris(1-methylethyl)- [aka 1,3,5-triisopropylbenzene]	6.36	Rainbow trout	0.30	24	0.50	1.14E+00
Benzo(b)fluorene	5.77	Rainbow trout	0.24	5	0.50	1.87E+00
Benzo(b)fluorene	5.77	Rainbow trout	0.17	24	0.50	3.33E+00
Benzo(ghi)perylene	6.63	Rainbow trout	0.09	24	0.50	7.56E+00
Benzo(k)fluoranthene	6.11	Rainbow trout	0.07	5	0.50	1.04E+01
Benzo(k)fluoranthene	6.11	Rainbow trout	0.20	24	0.50	2.56E+00
Benzo[a]pyrene	6.13	Rainbow trout	0.02	10	0.50	3.49E+01
Benzo[a]pyrene	6.13	Rainbow trout	0.49	20	0.50	4.71E-02
Benzo[a]pyrene	6.13	Rainbow trout	0.34	20	0.50	8.21E-01
Benzo[a]pyrene	6.13	Rainbow trout	0.14	20	0.50	4.37E+00
Benzo[a]pyrene	6.13	Rainbow trout	0.11	20	0.50	6.01E+00
Benzo[a]pyrene	6.13	Rainbow trout	0.07	20	0.50	1.04E+01
Benzo[b]chrysene	6.54	Rainbow trout	0.04	24	0.50	1.91E+01
Beta - Hexabromocyclododecane	5.47	Rainbow trout	0.41	31	0.51	4.01E-01
C10 perfluorodecylphosphonate	5.74	Rainbow trout	0.16	32	0.50	3.64E+00
C6 perfluorohexylphosphonate	3.06	Rainbow trout	0.05	32	0.50	1.39E+01
C6/C6 bis(perfluorohexyl)phosphinate	6.96	Rainbow trout	0.34	32	0.49	7.37E-01
C6/C8 perfluorohexylperfluorooctylphosphinate	8.30	Rainbow trout	0.24	32	0.28	2.56E-01
C8 perfluorooctylphosphonate	4.40	Rainbow trout	0.07	32	0.51	1.04E+01
Chrysene	5.81	Rainbow trout	0.29	5	0.50	1.26E+00
Chrysene	5.81	Rainbow trout	0.03	24	0.50	2.65E+01
Chrysene	5.81	Rainbow trout	0.05	10	0.50	1.56E+01
cis-1,1,3,5 Tetramethyl cyclohexane	4.88	Rainbow trout	0.40	24	0.51	4.55E-01
cis-Bicyclo[4.3.0]nonane	3.71	Rainbow trout	0.30	24	0.50	1.16E+00
Cyclohexane, 1,1'-(1,2-EthaneDiyl)Bis-	6.85	Rainbow trout	0.29	5	0.49	1.18E+00
Cyclohexylbiphenyl	6.57	Rainbow trout	0.37	5	0.50	5.94E-01
Cyproconazole	2.90	Rainbow trout	0.18	14	0.49	2.86E+00
Decabromodiphenyl ether	8.70	Zebrafish	0.01	28	0.17	3.45E+01
Decylbenzene	7.35	Rainbow trout	0.36	5	0.47	4.85E-01
Dehydroabietine	6.43	Rainbow trout	0.04	24	0.50	1.92E+01
Dibenzo[a,h]anthracene	6.54	Rainbow trout	0.02	24	0.50	3.99E+01
Diisoheptyl phthalate	7.41	Rainbow trout	0.32	5	0.46	7.18E-01

Chemical name	Log Kow	Species	Measured E_D	Ref.	Modelled E_D	Estimated k_R/d
Di-Me & Et naphthalenes	4.42	Rainbow trout	0.48	5	0.51	9.21E-02
endosulfan - α isomer	3.83	Atlantic salmon	0.21	33	0.50	2.37E+00
endosulfan - β isomer	3.83	Atlantic salmon	0.41	33	0.50	3.96E-01
Fipronil	4.01	Rainbow trout	0.28	22	0.50	1.37E+00
Fipronil	4.01	Rainbow trout	0.23	22	0.50	2.03E+00
Flouranthene	5.16	Rainbow trout	0.07	5	0.51	1.04E+01
Fluoranthene	5.16	Rainbow trout	0.30	24	0.51	1.17E+00
Fluoranthene	5.16	Rainbow trout	0.30	24	0.51	1.17E+00
Gamma - Hexabromocyclododecane	5.80	Rainbow trout	0.46	31	0.50	1.68E-01
Hexabromocyclododecane + α isomer	5.38	Zebrafish	0.50	34	0.51	7.66E-03
Hexabromocyclododecane + β isomer	5.47	Zebrafish	0.49	34	0.51	4.67E-02
Hexabromocyclododecane + β isomer	5.47	Zebrafish	0.34	34	0.51	8.48E-01
Hexabromocyclododecane + γ isomer	5.80	Zebrafish	0.39	34	0.50	5.29E-01
Hexabromocyclododecane α isomer	5.38	Zebrafish	0.41	34	0.51	4.09E-01
Hexabromocyclododecane - α isomer	5.38	Zebrafish	0.29	34	0.51	1.27E+00
Hexabromocyclododecane β isomer	5.47	Zebrafish	0.48	34	0.51	1.03E-01
Hexabromocyclododecane β isomer	5.47	Zebrafish	0.34	34	0.51	8.63E-01
Hexabromocyclododecane - β isomer	5.47	Zebrafish	0.31	34	0.51	1.09E+00
Hexabromocyclododecane γ isomer	5.80	Zebrafish	0.41	34	0.50	4.08E-01
Hexabromocyclododecane γ isomer	5.80	Zebrafish	0.29	34	0.50	1.23E+00
Hexabromocyclododecane - γ isomer	5.80	Zebrafish	0.29	34	0.50	1.26E+00
Hexabromocyclododecane - γ isomer	5.80	Zebrafish	0.16	34	0.50	3.54E+00
Hexadecahydropyrene	5.94	Rainbow trout	0.30	24	0.50	1.16E+00
Indeno 1,2,3-cd pyrene	6.70	Rainbow trout	0.08	24	0.50	8.67E+00
iso-butylcyclohexane	4.99	Rainbow trout	0.40	24	0.51	4.55E-01
Isodecanol (high dose)	3.57	Rainbow trout	0.34	5	0.50	8.18E-01
Isodecanol (low dose)	3.57	Rainbow trout	0.20	5	0.50	2.56E+00
isopropyl hydrophenanthrene (Fichtelite)	6.54	Rainbow trout	0.12	24	0.50	5.29E+00
Isotridecanol (high dose)	5.11	Rainbow trout	0.13	5	0.51	4.87E+00
Isotridecanol (low dose)	5.11	Rainbow trout	0.12	5	0.51	5.41E+00
Isoundecanol ethoxylate (11-3EO)	3.31	Rainbow trout	0.23	5	0.50	1.99E+00
m-Dicyclohexylbenzene	7.63	Rainbow trout	0.07	5	0.43	8.21E+00
Metconazole	3.85	Rainbow trout	0.40	14	0.50	4.54E-01
Methylnaphthalenes	3.86	Rainbow trout	0.43	5	0.50	2.98E-01
m-terphenyl	5.52	Rainbow trout	0.47	5	0.51	1.30E-01

Chemical name	Log Kow	Species	Measured E_D	Ref.	Modelled E_D	Estimated k_R/d
Myclobutanil	2.94	Rainbow trout	0.09	14	0.49	7.65E+00
n - Octyl Cyclohexane	7.03	Rainbow trout	0.05	5	0.49	1.61E+01
N,N'-Di-2-naphthyl-p-phenyleneDiamine	6.39	Common carp	0.19	23	0.50	2.76E+00
Naphthalene	3.30	Rainbow trout	0.04	24	0.50	1.92E+01
n-dodecane	6.10	Rainbow trout	0.22	5	0.50	2.18E+00
n-dodecane	6.10	Rainbow trout	0.10	24	0.50	6.77E+00
n-heptylcyclohexane	6.54	Rainbow trout	0.11	5	0.50	5.92E+00
n-Hexadecane (deuterated)	8.20	Rainbow trout	0.17	24	0.31	1.21E+00
n-hexyl cyclohexane	6.05	Rainbow trout	0.13	5	0.50	4.84E+00
n-hexyl cyclohexane	6.05	Rainbow trout	0.14	10	0.50	4.37E+00
n-nonane	5.65	Rainbow trout	0.13	24	0.51	4.86E+00
n-octyl benzene	6.30	Rainbow trout	0.04	5	0.50	1.93E+01
n-octyl benzene	6.30	Rainbow trout	0.20	24	0.50	2.55E+00
n-Tetradecane	7.20	Rainbow trout	0.38	5	0.48	4.48E-01
n-tridecane	6.73	Rainbow trout	0.20	24	0.50	2.48E+00
Octachlorodibenzofuran	8.60	Guppy	0.02	13	0.20	1.06E+01
Octachlorodibenzofuran	8.60	Guppy	0.02	13	0.20	1.61E+01
Octachlorodibenzofuran	8.60	Guppy	0.01	13	0.20	2.78E+01
Octachlorodibenzofuran	8.60	Guppy	0.01	13	0.20	4.23E+01
Octachlorodibenzofuran	8.60	Guppy	0.003	13	0.20	8.60E+01
Octamethylcyclotetrasiloxane	6.74	Rainbow trout	0.40	35	0.50	4.07E-01
o-Terphenyl	5.52	Rainbow trout	0.09	5	0.51	7.75E+00
o-Terphenyl	5.52	Common carp	0.43	23	0.51	3.02E-01
o-Terphenyl	5.52	Rainbow trout	0.30	24	0.51	1.17E+00
o-Terphenyl	5.52	Rainbow trout	0.45	20	0.51	2.12E-01
o-Terphenyl	5.52	Rainbow trout	0.43	20	0.51	3.02E-01
o-Terphenyl	5.52	Rainbow trout	0.30	20	0.51	1.17E+00
o-Terphenyl	5.52	Rainbow trout	0.29	20	0.51	1.27E+00
o-Terphenyl	5.52	Rainbow trout	0.23	20	0.51	2.03E+00
o-Terphenyl	5.52	Rainbow trout	0.23	20	0.51	2.03E+00
o-Terphenyl	5.52	Common carp	0.17	20	0.51	3.33E+00
perhydro-chrysene	6.24	Rainbow trout	0.18	24	0.50	3.02E+00
Phenanthrene	4.46	Rainbow trout	0.08	24	0.51	8.93E+00
Propiconazole	3.72	Rainbow trout	0.13	14	0.50	5.04E+00
syn-Dechlorane Plus	9.00	Rainbow trout	0.06	30	0.10	8.72E-01

Chemical name	Log Kow	Species	Measured E_D	Ref.	Modelled E_D	Estimated k_R /d
t-decalin	4.79	Rainbow trout	0.34	24	0.51	8.34E-01
t-decalin	4.79	Rainbow trout	0.19	10	0.51	2.81E+00
Tebuconazole	3.70	Rainbow trout	0.28	14	0.50	1.39E+00
Tetraconazole	3.56	Rainbow trout	0.09	14	0.50	7.65E+00
Triadimefon	2.77	Rainbow trout	0.25	14	0.49	1.56E+00
Tri-Me naphthalenes	4.73	Rainbow trout	0.32	5	0.51	9.92E-01
Triphenylene	5.49	Rainbow trout	0.17	5	0.51	3.42E+00
Triphenylene	5.49	Rainbow trout	0.50	24	0.51	1.84E-02
Tris(4-chlorophenyl)methane	7.30	Rainbow trout	0.25	16	0.47	1.45E+00
α -Hexabromocyclododecane	5.38	Rainbow trout	0.31	31	0.51	1.08E+00

ESI – 6: BCFBAF BAF-QSAR model simulations

Figure ESI-3 illustrates the BAF-QSAR model predictions for an upper trophic level fish for a range of hypothetical hydrophobic chemicals (K_{OW}) and a range of assumed k_B and k_R values. Commonly used bioaccumulation hazard criteria of 5,000 L/kg-ww and 1,000 L/kg-ww are included for referencing the combination of chemical properties that result in different bioaccumulation hazard classifications. The inclusion of the new E_D model results in higher BAFs for super-hydrophobic chemicals compared to BAFs calculated with the original E_D regression model³⁶ included in the BAF-QSAR³⁷. In these illustrations we did not re-calibrate the BAF-QSAR model to the measured BAF database³⁷ but that should be done if the new E_D model is included for BAF predictions for decision-making to account for possible changes in the overall food web biomagnification factor resulting from including the new E_D model. There were however no measured BAF data for chemical with $\log K_{OW} > 8.2$ in the original calibration dataset and this is around the range of K_{OW} in which the models differ as a result of changes to the E_D sub-model. The only difference in model output between Figure ESI-3A and ESI-3B is that degradation rates in the GIT (k_R) are also considered in Fig ESI-3B. In these examples k_{RS} are assumed equal to $k_{B,NS}$ for most simulations. As rates of biotransformation and degradation increase from values of zero the BAFs drop at higher K_{OW} and this has been demonstrated before, e.g.,^{38, 39}. Differences in the screening-level BAF calculations when $k_R \sim k_{B,N}$ are minimal. When $k_{B,N}$ is about 0.5 /day, all of the BAFs are below the criterion of 1,000. When $k_{B,N}$ is 0.1 /d, k_R has to be about 100 times faster ($k_R \sim 10$ /d) for the BAF to drop below 5,000 for all chemicals.

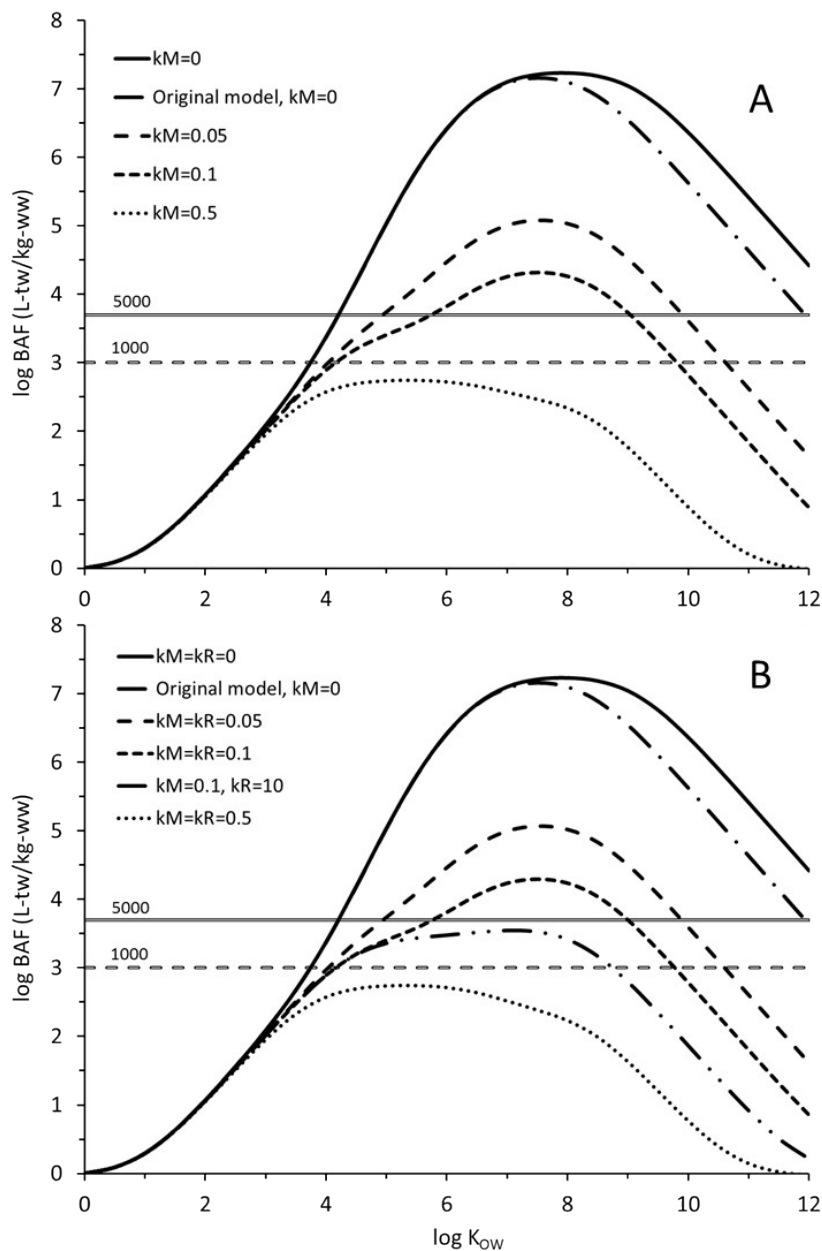


Figure ESI-3: BAF-QSAR model simulations for an upper trophic level fish as a function of the octanol-water partition coefficient (K_{OW}). (A) Various assumptions for fish biotransformation rate constants $k_{B,N}$ (aka k_M) ranging from 0 to 0.5 /d; degradation in GIT assumed negligible and (B) various assumptions for degradation rate constants in the GIT k_R , i.e., $k_R = k_{B,N}$ and $k_R = 100 k_{B,N}$. BAF criteria of 1,000 and 5,000 L-total water/kg-wet weight are also presented. Modelled BAFs are based on total water concentrations (dissolved and sorbed).

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