Supporting Information for

Transformation of Chiral Polychlorinated Biphenyls (PCBs) in a Stream Food Web.

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Supporting Information for determining the effect of interfering congeners.

We evaluated the co-elution for our studies by applying the Frame (*1*) approach to the calibration standard that we used (1:1:1 mixture of Aroclors 1016, 1254, and 1260). Using the conditions listed in the manuscript, congeners 84, 91, and 136 do not coelute with any other congeners, while PCB 95 coelutes with 66, PCB 149 coelutes with 130 and 123, and PCB 174 coelutes with 197 and 202. However, congeners 197 and 202 are not present in our samples. In the calibration mixture, the weight percent contribution of 130 and 123 is 12 times lower than the weight percent of 149; therefore, we assumed that the interference due to co-elution is negligible. Conversely, the weight percent contribution of 66 is only 2.5 times lower than the contribution of 95 and we verified that 66 is also not an interference by analysis with GC-MS.

To validate the assumption that interfering congeners are not an issue in our case, chiral signatures of PCB 95 were measured with a Varian (4000 GC/MS/MS), which is an ion trap mass spectrometer instrument and the GC/MS instrument available to our research group. The instruments used by references (*2-4*) as well as by Robson and Harrad (*5*) were quadrupole MS instruments. Our GC operation was based on Selected Ion Storage (SIS) mode with the ion trap mass spectrometer detector using the same Chirasil-Dex column as used with the GC/ECD. A working standard of PCB 95 was injected into the GC/MS to determine retention time, ratio of m/z of two enantiomers, and EF value. The value of m/z was the same as that identified by Hall (*2*) and the EF value was close to 0.5. A series of diluted solution was also analyzed to quantify a detection limit prior to sample analysis. Because the detection limit for this method is approximately >0.1ppm, we selected the SPMD samples, which have the highest concentrations of our study. Results confirmed that racemic EFs of PCB 95 were observed, which is similar to the results on the GC/ECD and Chirasil-Dex. Therefore, we verified our assumption that 66 is not an interference by analysis with GC/MS.

Figure S1. Map of the study area showing the Sangamo-Weston plant (SW) and four collection sites: 2, 3, 4, and 6. Open circle designates Asian clam collection site. Solid rectangular represents contamination source, the Sangamo-Weston plant, which is located on the Twelvemile Creek tributary, 39 km upstream from the top of the lake. Solid arrow indicates direction of river flow.

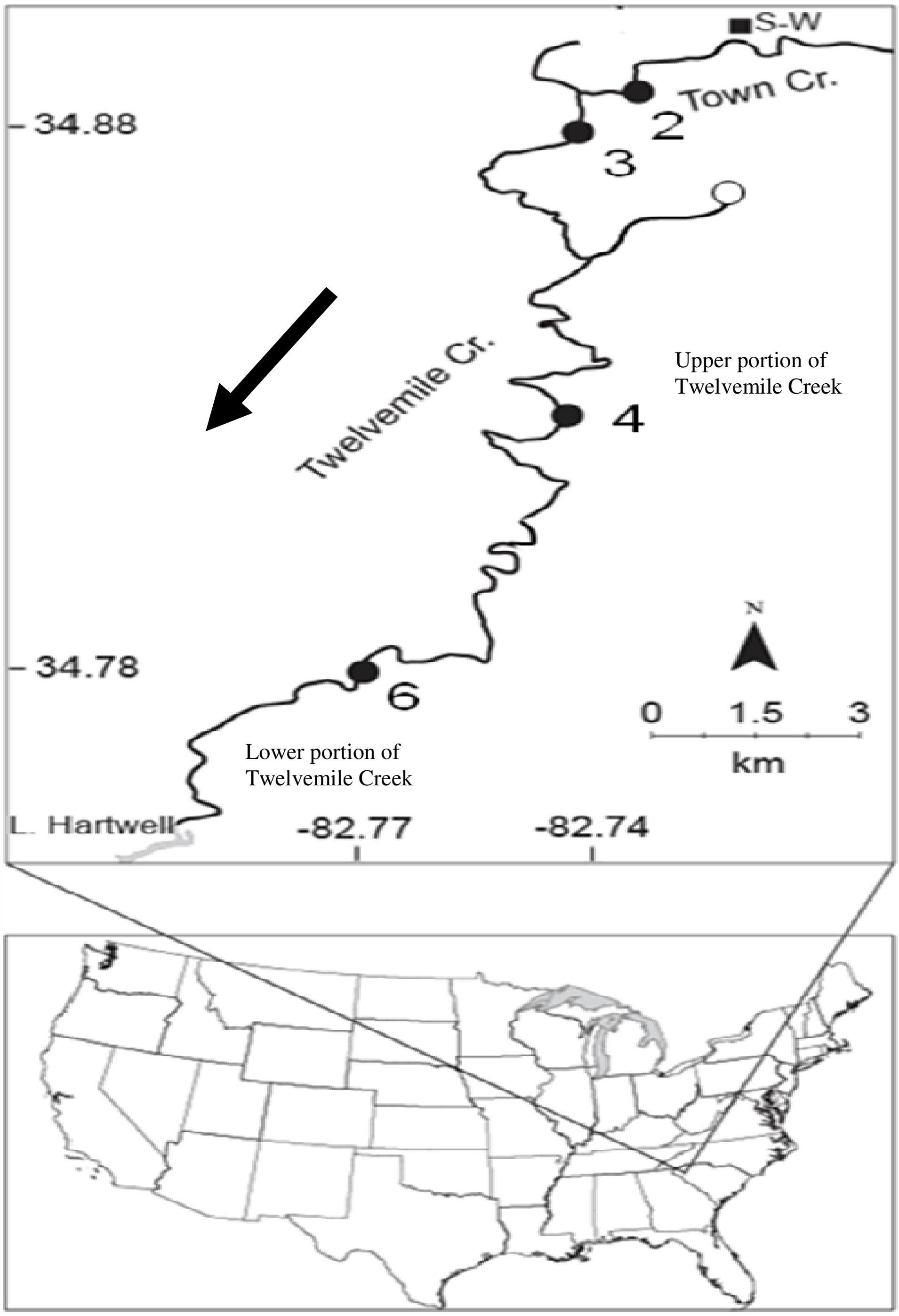

Figure S2. EFs variation of PCB 91 among four sites in Twelvemile Creek matrices. EFs were measured at two sites for mayfly, yellowfin shiner, three sites for CPOM, and four sites for FBOM and SPMD. EFs of PCB 91 were not observed in sediment, periphyton, and Asian clam. EFs measured in matrices among sites were not statistically different (Tukey test, P< 0.05), except for EFs of PCB 91 in yellowfin shiner.

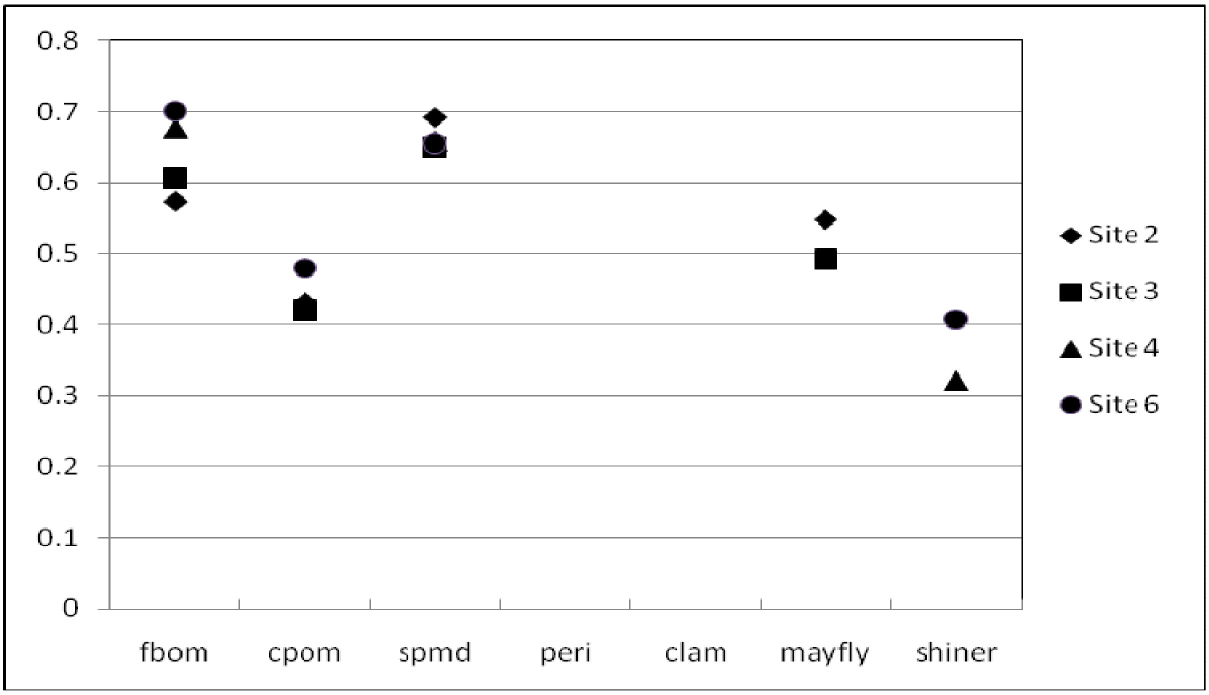

Figure S3. EFs variation of PCB 95 among four sites in Twelvemile Creek matrices. The EF values were measured at two sites for mayfly, three sites for CPOM, periphyton, Asian clams, and four sites for FBOM, SPMD, and yellowfin shiner. EFs of PCB 95 were not measured in sediments. EFs measured in matrices among sites were not statistically different (Tukey test, P< 0.05)

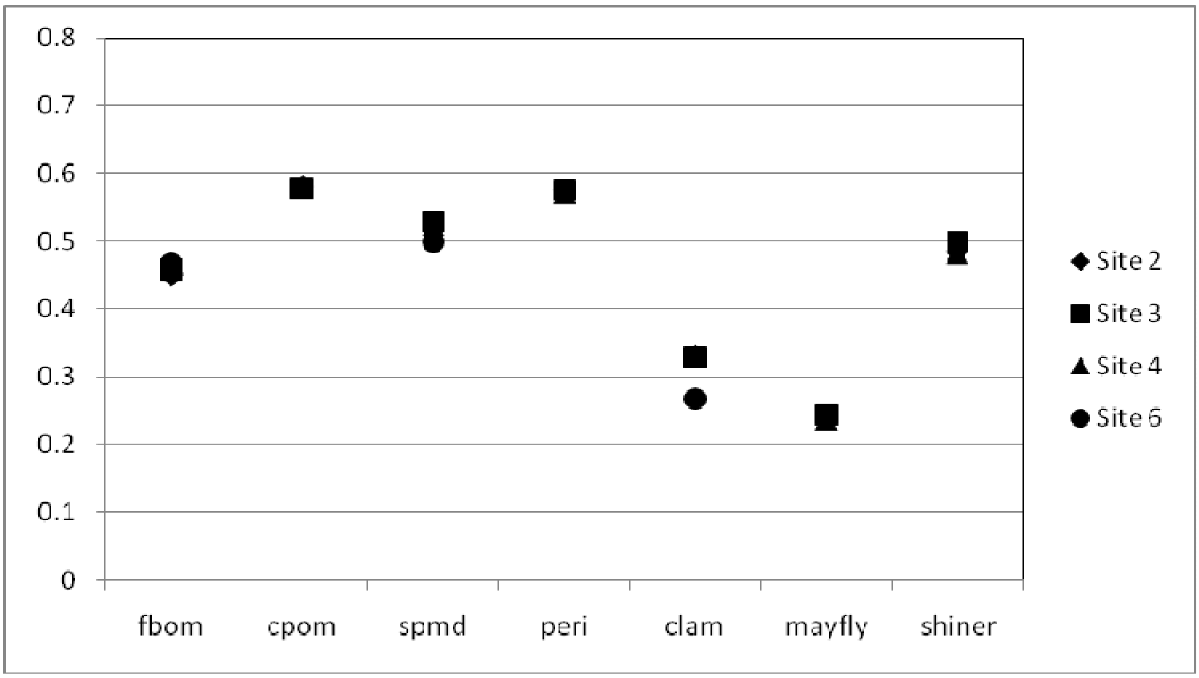

Figure S4. EFs variation of PCB 136 among four sites in Twelvemile Creek matrices. The EF values were measured at two sites for CPOM, three sites for periphyton, and four sites for FBOM, SPMD, Asian clams, and yellowfin shiner. EFs of PCB 136 were not measured in sediment and mayfly. The EFs measured in matrices were not statistically different (Tukey test. P<0.05), except for EFs of PCB 136 in Asian clams.

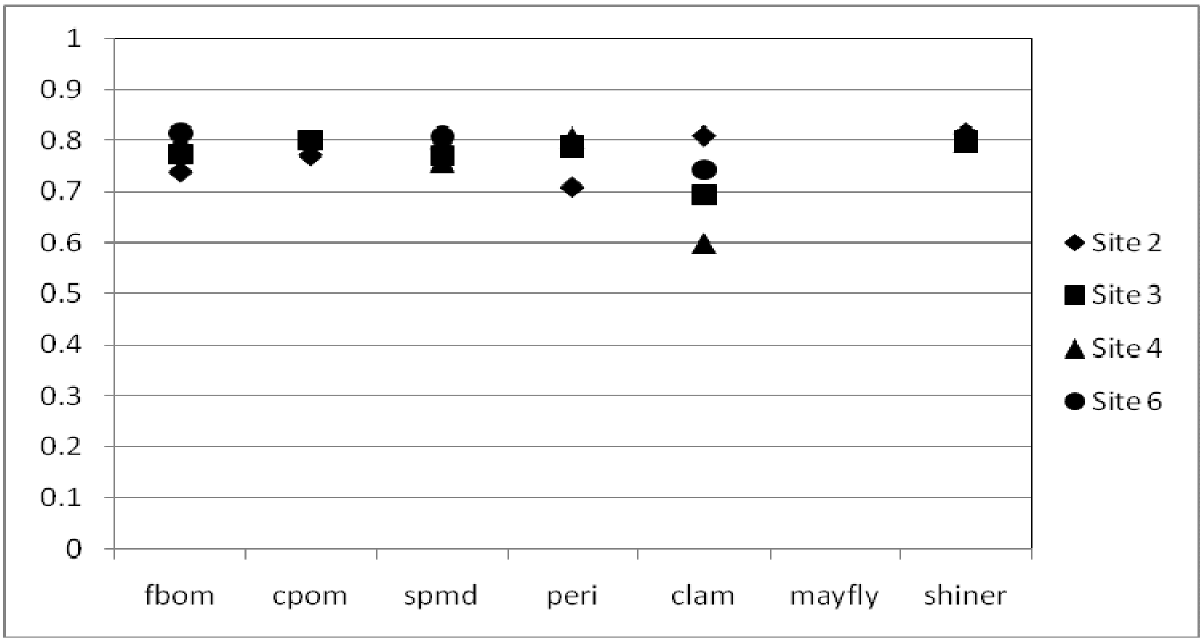

Figure S5. EF variations of PCB 149 amoung four sites in Twelvemile Creek matrices. EFs were measured at two sites for periphyton, three sites for CPOM, and four sites for FBOM, SPMD, Asian clam, mayfly, and yellowfin shiner. EFs of PCB 149 were not observed in sediment at all four sites. The EFs measured in matrices were not statistically different (Tukey test, P< 0.05).

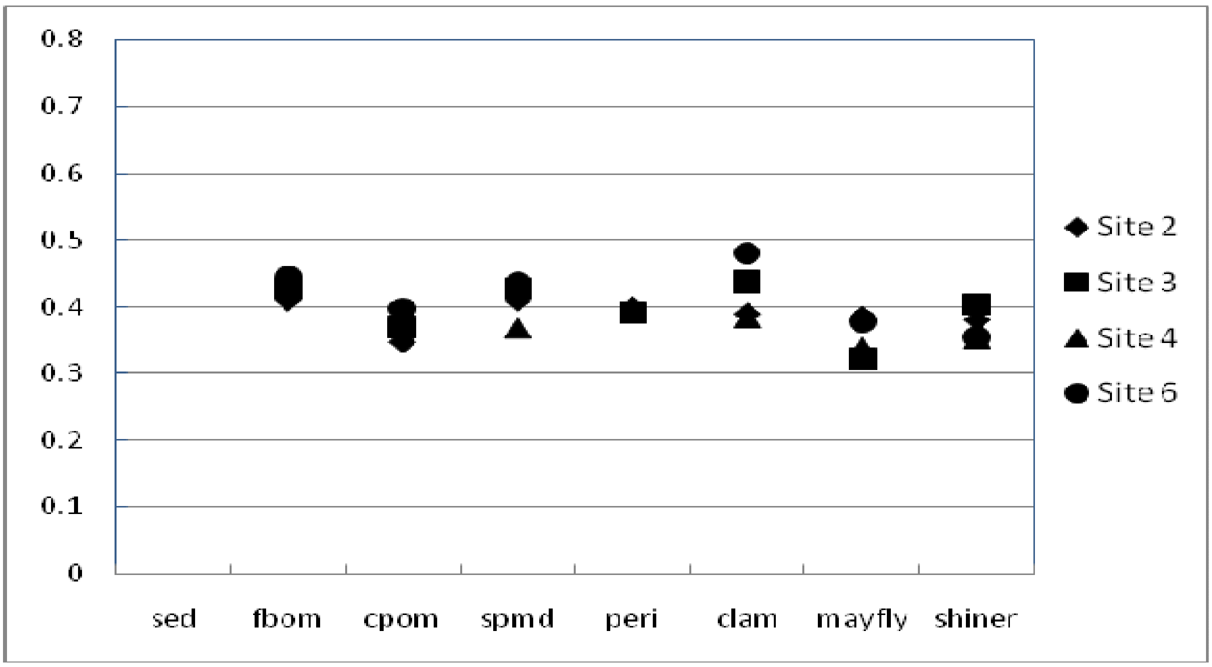

Table S1. Total PCB concentrations (mean ± 1 SD, µg/g wet mass or µg/g lipid for SPMD) in Twelvemile Creek matrices. Concentrations of SPMD and Asian clam are average concentrations measured in 10, 24, 40, and 60-d.

Media	Site 2	Site 3	Site 4	Site 6
Sediment	0.02	0.02	0.03	0.03
FBOM	0.79 ± 0.36	0.16 ± 0.13	0.15 ± 0.10	0.24 ± 0.16
CPOM	0.23 ± 0.19	0.19 ± 0.11	0.14 ± 0.03	0.16 ± 0.06
Periphyton	0.19 ± 0.06	0.16 ± 0.03	0.28 ± 0.08	0.23 ± 0.02
SPMD	4.26 ± 1.79	1.87 ± 1.01	1.22 ± 0.16	1.95 ± 0.84
Asian clam	0.19 ± 0.03	0.07 ± 0.01	0.07	0.04
Mayfly	0.75 ± 0.69	0.19 ± 0.02	0.34 ± 0.05	0.27 ± 0.04
Yellowfin shiner	2.43 ± 0.17	2.68 ± 0.18	1.87 ± 0.16	2.12 ± 0.16

Table S2. Concentrations (mean ± 1 SD, ng/g wet mass or ng/g lipid for SPMD) of chiral PCB congeners in Twelvemile Creek matrices . Concentrations of congeners in SPMD and Asian clam were average concentrations measured in 10, 24, 40, and 60-d.

Media	N	PCB 84	PCB 91	PCB 95	PCB 136	PCB 149	PCB 174
Sediment	12	BDL	BDL	BDL	BDL	BDL	BDL
FBOM	15	8.04 ± 6.84	4.80 ± 3.25	16.4 ± 7.96	1.62 ± 0.29	17.0 ± 9.61	BDL
CPOM	24	BDL	5.46 ± 2.81	2.65 ± 1.14	BDL	5.29 ± 3.10	BDL
Periphyton	26	BDL	BDL	BDL	1.62 ± 0.67	8.60 ± 4.41	BDL
SPMD	42	18.0 ± 12.2	7.22 ± 3.57	119 ± 61.7	BDL	18.4 ± 11.4	BDL
Asian clam	33	BDL	1.35 ± 0.61	2.67 ± 1.01	BDL	1.45 ± 0.75	BDL
Mayfly	12	BDL	2.36 ± 0.87	13.4 ± 4.87	BDL	4.92 ± 4.09	BDL
Yellowfin shiner	12	BDL	13.5 ± 1.82	BDL	2.80 ± 0.47	43.2 ± 8.42	5.82 ± 0.98

N: number of samples analyzed in this study. BDL: below detection limit.

Table S3. EF values (mean ± 1 SD) of chiral PCB congeners in Twelvemile Creek matrices.EFs for SPMD and Asian clam in each site were average EFs measured in 10, 24, 40, and 60-d

Media	PCB 84	PCB 91	PCB 95	PCB 136	PCB 149	PCB 174
Sediment	ND	ND	ND	ND	ND	ND
FBOM	0.45 ± 0.03*	0.63 ± 0.05*	0.46 ± 0.01*	0.77 ± 0.03*	0.43 ± 0.02*	ND
CPOM	ND	0.47 ± 0.07*	0.58 ± 0.03*	0.78 ± 0.04**	0.37 ± 0.04*	ND
Periphyton	ND	ND	ND	0.41 ± 0.02	0.39 ± 0.04***	ND
SPMD	0.45 ± 0.04*	0.67 ± 0.03*	0.517 ± 0.03*	0.79 ± 0.03*	0.42 ± 0.04*	ND
Asian clam	0.60 ± 0.07**	ND	0.30 ± 0.04**	0.71 ± 0.08*	0.42 ± 0.05*	ND
Mayfly	ND	0.51 ± 0.03***	0.24 ± 0.03***	0.80 ± 0.01***	0.35 ± 0.04*	ND
Yellowfin shiner	ND	0.33 ± 0.09***	0.49 ± 0.02*	0.80 ± 0.01*	0.37 ± 0.03*	0.51 ± 0.01*

*: indicates EFs measured at all four sites. **: indicates EFs measured at three sites. ***: indicates EFs measured at two sites. There was no statistical difference in EFs measured among sites and among deployment times for SPMD and Asian clams (Tukey test, $P<0.05$).

Literature cited

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