Supplementary Information for the article;

Quantitative Thermodynamic Exposure Assessment (QTEA) of PCBs available to Sandworms (*Alitta virens*) in Activated Carbon Remediated Sediment during Ongoing Sediment Deposition

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Content of the Supporting Information

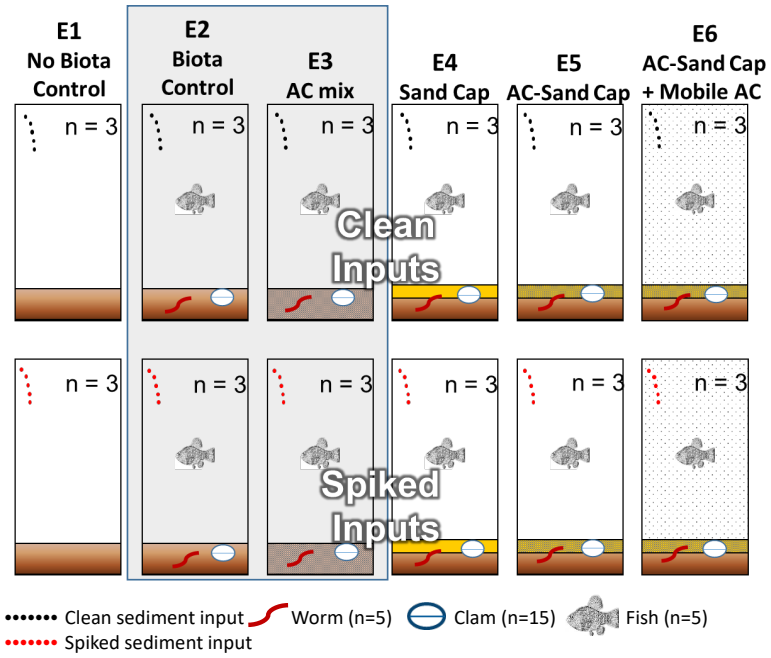

Figure S1. Full experimental design of the larger investigation showing all mesocosms (E1 to E6). Biota "control" (E2) and "AC mix" (E3) were the focus of this publication. Other results from the larger investigation have been published in Schmidt et al. (2017), Gidley et al. (2019, 2022), and Bridges et al. (2022).

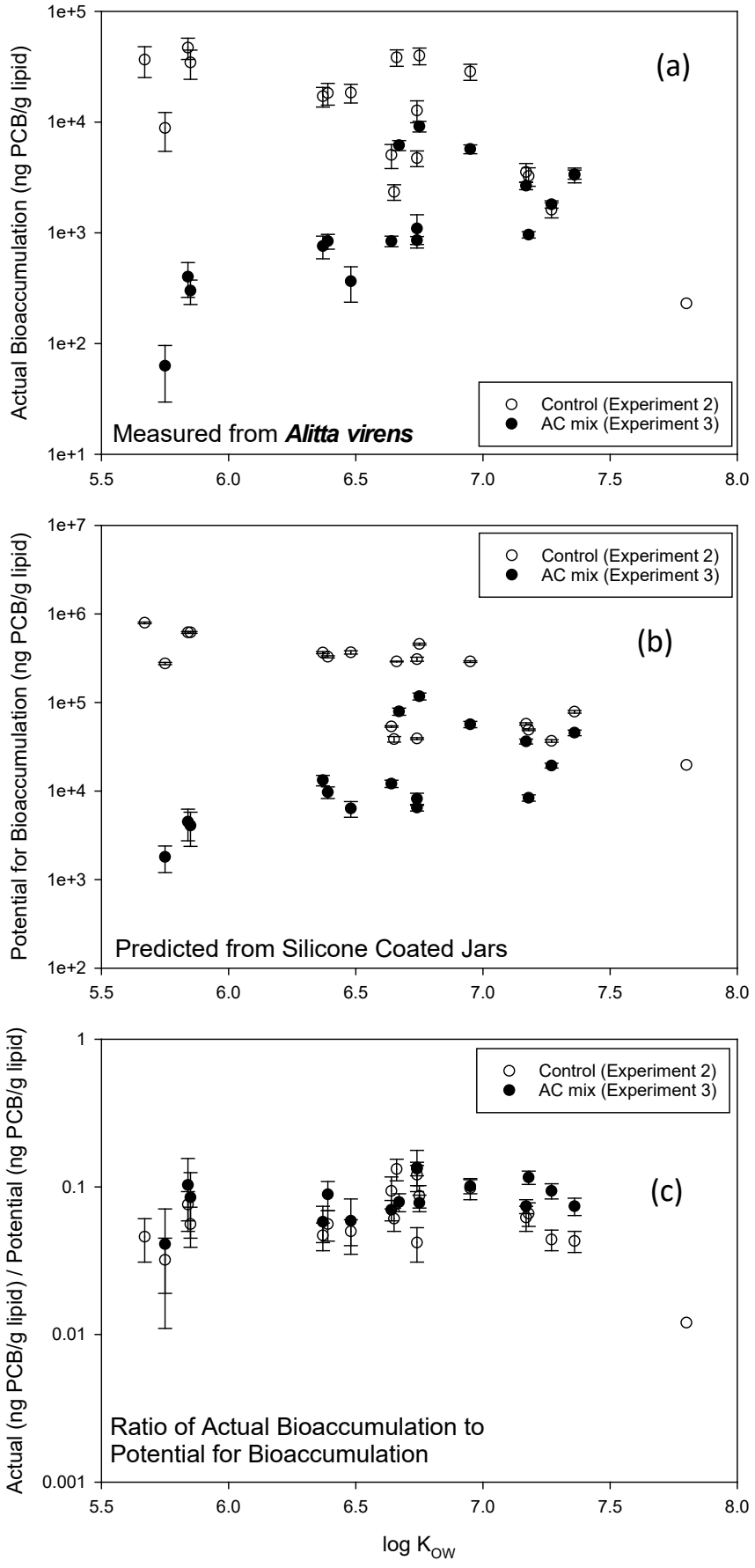
Actual Bioaccumulation (ng PCB/g lipid)
1e+5
1e+4
1e+3
1e+2
1e+1
(a)
Control (Experiment 2)
AC mix (Experiment 3)
Measured from Alitta virens
5.5
6.0
6.5
7.0
7.5
8.0
Potential for Bioaccumulation (ng PCB/g lipid)
1e+7
1e+6
1e+5
1e+4
1e+3
1e+2
(b)
Control (Experiment 2)
AC mix (Experiment 3)
Predicted from Silicone Coated Jars
Actual (ng PCB/g lipid) / Potential (ng PCB/g lipid)
1
0.1
0.01
0.001
(c)
Control (Experiment 2)
AC mix (Experiment 3)
Ratio of Actual Bioaccumulation to
Potential for Bioaccumulation
log K_OW

Figure S2. PCB congeners actually measured in worm lipid (a), “predicted” in lipid based on sediment ESDs (b), and the ratio of values in Figure S2a and Figure S2b all versus log K_{OW} (Hawker and Connell 1988). Figure S2 averages across spiked and clean inputs, but compares AC mix versus untreated control. Figure S2 also shows the decrease in concentrations by AC tended to be lower for more hydrophobic PCBs, indicating lower remediation efficacy. Error bars show one standard deviation (SD) of the mean (n = 6).

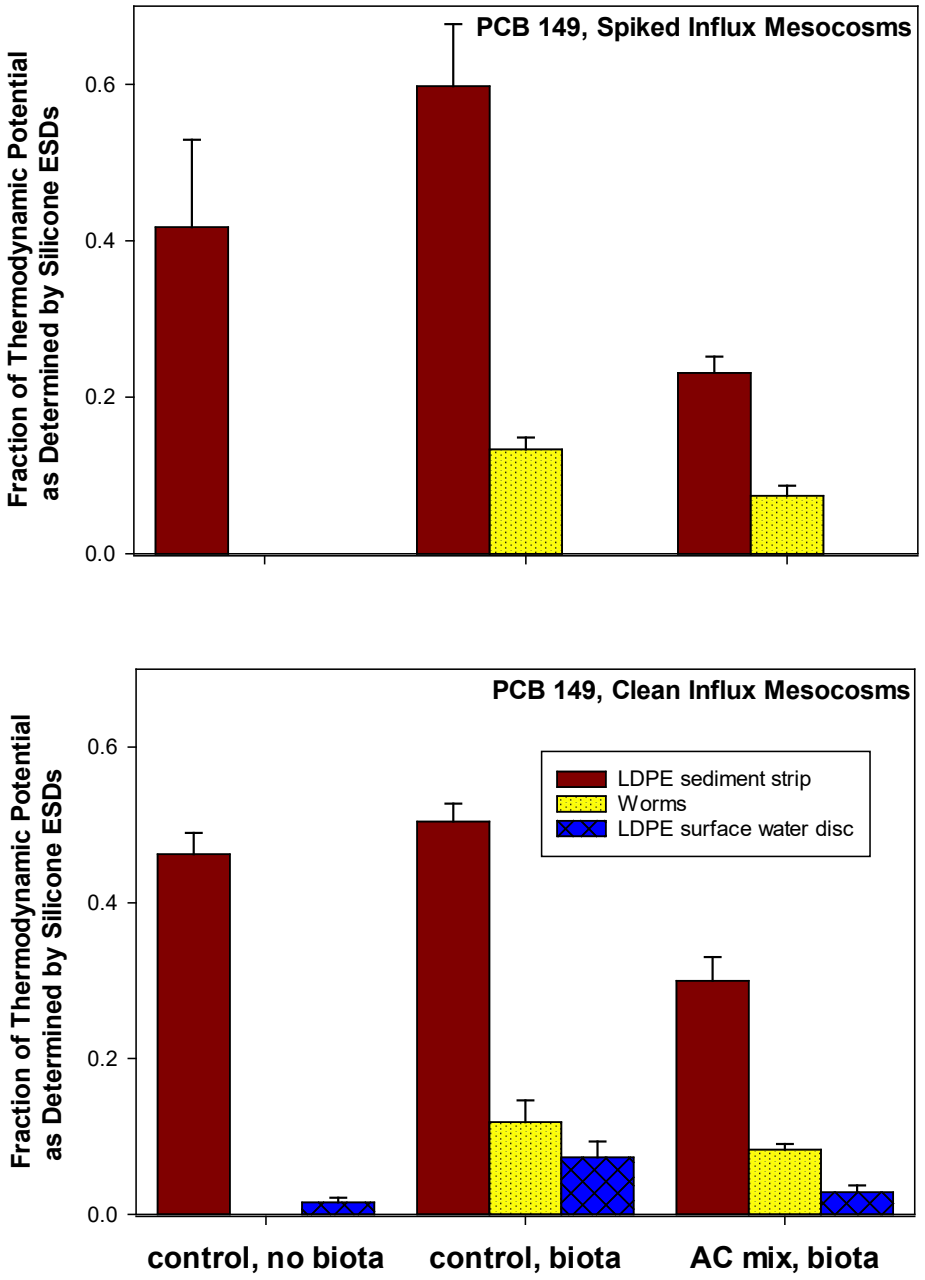

Figure S3. Fraction of thermodynamic potential as defined by silicone equilibrium sampling devices (ESDs) (similar to Figure 3 in the article). Silicone ESDs sampled surficial bed sediment. *In situ* low density polyethylene (LDPE) strips sampled surficial bed sediment. *In situ* LDPE discs sampled surface water (overlying water). LDPE discs are not shown in the spiked influx mesocosms. Error bars show one standard deviation of the mean (n=3).

Table S1. Polymer-lipid partition coefficients (K_{PL}) applied in the present study (derived from Gilbert et al. (2016) for silicone and Smedes et al. (2017) for LDPE).

Congener	Co-elute	Co-elute	K_{PL} (LDPE)	K_{PL} (Silicone)
18			0.0880	
28	31		0.1026	0.1157
44			0.0756	0.1756
49			0.0852	0.1189
52			0.0790	0.1263
77			0.0903	
81	117		0.1059	
99				0.0828
90	101			0.0838
105			0.0877	0.0925
110				0.1110
114			0.1096	
118			0.0952	0.0682
123			0.1003	
126	129		0.0878	
128				0.1282
138	163	164	0.0864	0.0809
149	147			0.0945
151				0.0991
132	153			0.0586
156	157		0.0952	0.0593
167			0.1034	
170			0.0860	0.0761
180			0.0995	0.0509
187			0.0978	0.0687

References

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