

SUPPORTING INFORMATION

Discovery of Hydroxylated Polychlorinated Biphenyls (OH-PCBs) in sediment from a Lake Michigan waterway and original commercial Aroclors

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Number of pages: 11

Number of figures: 3

Number of tables: 5

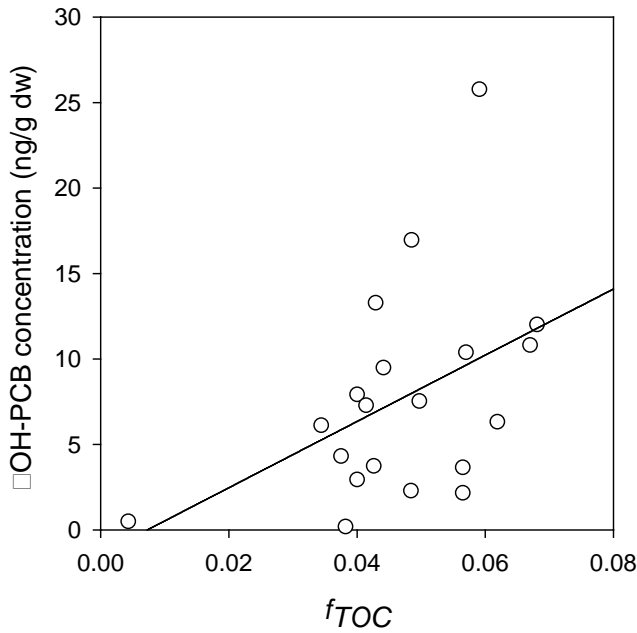


Figure S1. $\Sigma OH-PCB$ increases with increasing TOC ($R^2 = 0.20$, $p = 0.048$). Each circle represents a sample.

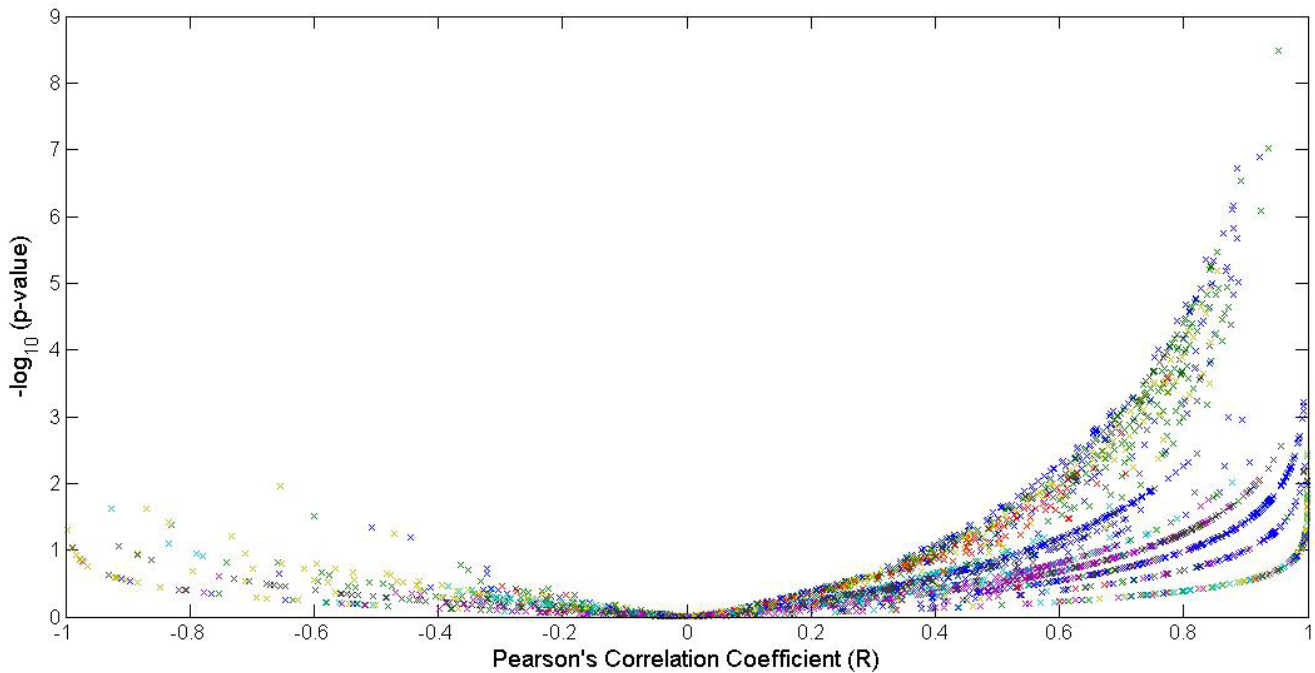


Figure S2. The Pearson's Correlation Coefficient and p-value for each OH-PCB:PCB pair. Each point on the graph represents one pair. Pairs were included only if both the OH-PCB and PCB were measured in at least 3 samples (2764 pairs). 713 pairs (26%) had significant relationships ($p < 0.05$). A positive R -value signifies a positive relationship (i.e. OH-PCB concentration increases as PCB concentration increases). Conversely, a negative R -value signifies a negative relationship (i.e. OH-PCB concentration decreases as PCB concentration increases). Of the statistically significant relationships, almost all (705 pairs) were positive.

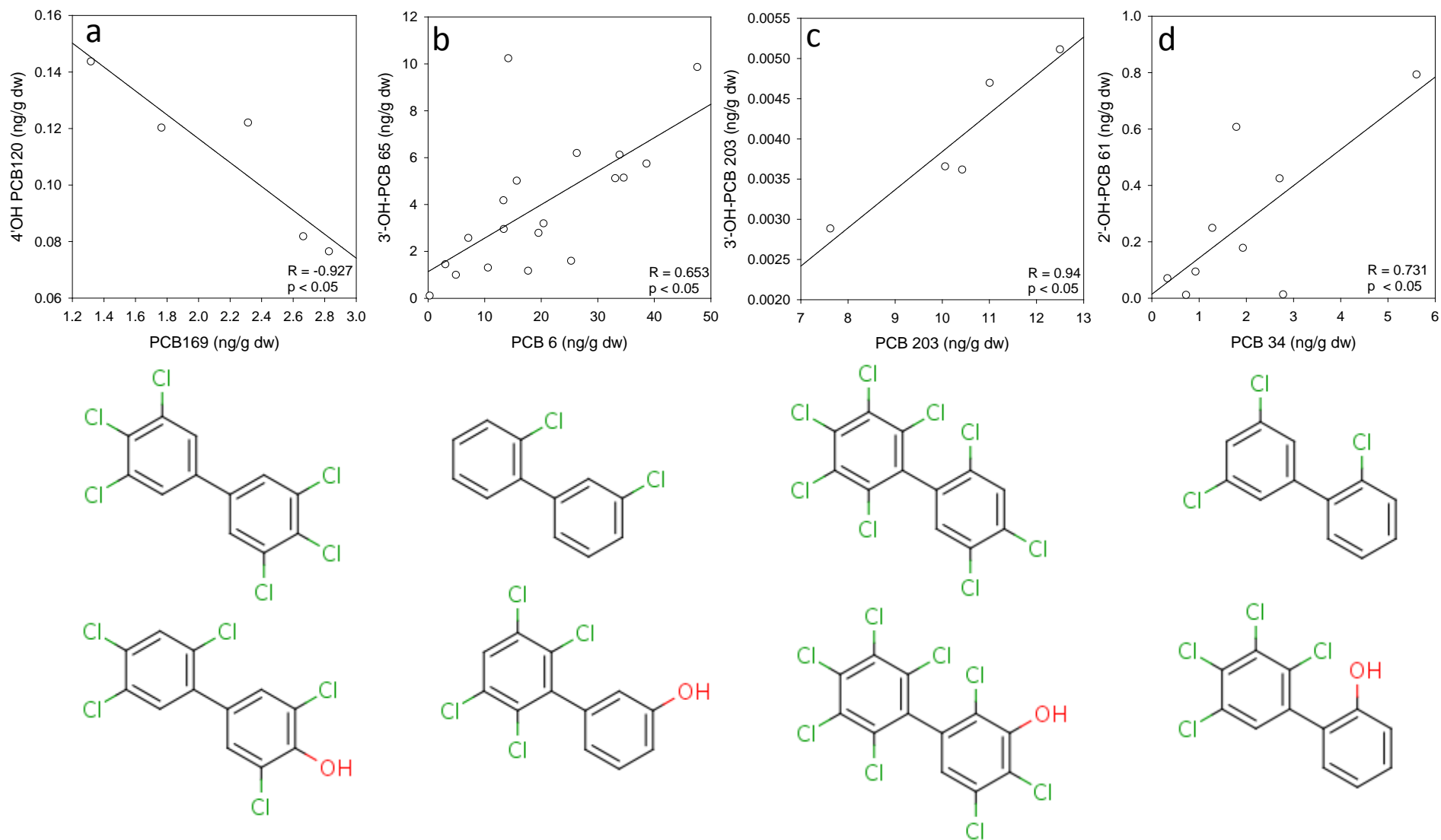


Figure S3. Significant correlations between OH-PCB:PCB pairs. Examples (a) and (b) involve OH-PCBs that were measured in both sediment and Aroclor. Assuming degradation refers to the possibility of dechlorination and insertion of an OH group but not chlorination or rearrangement of the chlorine atoms, neither OH-PCB could be formed from degradation of the PCB. Examples (c) and (d) involve OH-PCBs that were measured in sediment but not Aroclor. In example (c) the OH-PCB could be formed by degradation of the PCB but in example (d) the OH-PCB could not be formed by degradation of the PCB.

Table S1. Precursor and dominant product ions of the 65 quantitative calibration standards. The standards were purchased from either AccuStandard, Inc. (AccuStd) or Wellington Laboratories (Well).

Source	Congener	Abbreviation	Homolog	Precursor	Product
AccuStd	4-methoxy-2-chlorobiphenyl	4-MeO-PCB 1	mono	218.6	174.9
AccuStd	4-methoxy-3-chlorobiphenyl	4-MeO-PCB 2	mono	218.6	174.9
AccuStd	6-methoxy-3-chlorobiphenyl	6-MeO-PCB 2	mono	218.6	168
AccuStd	4'-methoxy-4-chlorobiphenyl	4'-MeO-PCB 3	mono	218.6	174.9
AccuStd	2'-methoxy-2,3-dichlorobiphenyl	2'-MeO-PCB 5	di	253.1	201.9
AccuStd	3'-methoxy-2,5-dichlorobiphenyl	3'-MeO-PCB 9	di	253.1	152
AccuStd	4'-methoxy-2,5-dichlorobiphenyl	4'-MeO-PCB 9	di	253.1	210.9
AccuStd	2'-methoxy-3,4-dichlorobiphenyl	2'-MeO-PCB 12	di	253.1	201.9
AccuStd	4-methoxy-3,5-dichlorobiphenyl	4-MeO-PCB 14	di	253.1	210.9
AccuStd	4'-methoxy-2,2',5-trichlorobiphenyl	4'-MeO-PCB 18	tri	287.5	245
AccuStd	4'-methoxy-2,3',5-trichlorobiphenyl	4'-MeO-PCB 26	tri	287.5	245
AccuStd	6'-methoxy-2,3',5-trichlorobiphenyl	6'-MeO-PCB 26	tri	287.5	238
AccuStd	2'-methoxy-2,4,6-trichlorobiphenyl	2'-MeO-PCB 30	tri	287.5	238
AccuStd	3'-methoxy-2,4,6-trichlorobiphenyl	3'-MeO-PCB 30	tri	287.5	245
AccuStd	4'-methoxy-2,4,6-trichlorobiphenyl	4'-MeO-PCB 30	tri	287.5	245
AccuStd	3-methoxy-2,2',6,6'-tetrachlorobiphenyl	3-MeO-PCB 54	tetra	322.0	278.8
AccuStd	2'-methoxy-2,3,4,5-tetrachlorobiphenyl	2'-MeO-PCB 61	tetra	322.0	272
AccuStd	3'-methoxy-2,3,4,5-tetrachlorobiphenyl	3'-MeO-PCB 61	tetra	322.0	221.8
WellMixA	4'-methoxy -2,3,4,5-tetrachlorobiphenyl	4'-MeO-PCB 61	tetra	322.0	278.8
AccuStd	2'-methoxy-2,3,5,6-tetrachlorobiphenyl	2'-MeO-PCB 65	tetra	322.0	272
AccuStd	3'-methoxy-2,3,5,6-tetrachlorobiphenyl	3'-MeO-PCB 65	tetra	322.0	221.8
AccuStd	4'-methoxy-2,3',4,6-tetrachlorobiphenyl	4'-MeO-PCB 69	tetra	322.0	278.8
AccuStd	6'-methoxy-2,3',4,6-tetrachlorobiphenyl	6'-MeO-PCB 69	tetra	322.0	272
AccuStd	4'-methoxy-2,3',5,5'-tetrachlorobiphenyl	4'-MeO-PCB 72	tetra	322.0	278.8
WellMixB	4'-methoxy-3,3',4,5'-tetrachlorobiphenyl	4'-MeO-PCB 79	tetra	322.0	278.8
AccuStd	6'-methoxy-2,2',3,3',5-pentachlorobiphenyl	6'-MeO-PCB 83	penta	356.4	305.8
AccuStd	4'-methoxy-2,2',3,4,5-pentachlorobiphenyl	4'-MeO-PCB 86	penta	356.4	312.9
AccuStd	4'-methoxy-2,2',3,5,6-pentachlorobiphenyl	4'-MeO-PCB 93	penta	356.4	312.9
WellMixG	4'-methoxy-2,2',3',4,5-pentachlorobiphenyl	4'-MeO-PCB 97	penta	356.4	312.9
WellMixB	4'-methoxy-2,2',4,5,5'-pentachlorobiphenyl	4'-MeO-PCB 101	penta	356.4	312.9
AccuStd	6'-methoxy-2,2',4,5,5'-pentachlorobiphenyl	6'-MeO-PCB 101	penta	356.4	305.8
AccuStd	6'-methoxy-2,3,3',4,5-pentachlorobiphenyl	6'-MeO-PCB 106	penta	356.4	305.8
WellMixF	4-methoxy-2,3,3',4',5-pentachlorobiphenyl	4-MeO-PCB 107	penta	356.4	312.9
WellMixE	4'-methoxy-2,3,3',4,5'-pentachlorobiphenyl	4'-MeO-PCB 108	penta	356.4	312.9
WellMixC	2-methoxy-2,3,4,4',5-pentachlorobiphenyl	2'-MeO-PCB 114	penta	356.4	305.8
WellMixD	3-methoxy-2,3',4,4',5-pentachlorobiphenyl	3-MeO-PCB 118	penta	356.4	312.9
WellMixA	4'-methoxy-2,3',4,5,5'-pentachlorobiphenyl	4'-MeO-PCB 120	penta	356.4	312.9
WellMixH	4'-methoxy-3,3',4,5,5'-pentachloro-biphenyl	4'-MeO-PCB 127	penta	356.4	340.7
WellMixE	4'-methoxy-2,2',3,3',4,5'-hexachlorobiphenyl	4'-MeO-PCB 130	hexa	390.9	346.8
WellMixB	4-methoxy-2,2',3,3',5,6-hexachlorobiphenyl	4-MeO-PCB 134	hexa	390.9	346.8
WellMixD	3'-methoxy-2,2',3,4,4',5'-hexachlorobiphenyl	3'-MeO-PCB 138	hexa	390.9	346.8
AccuStd	5-methoxy-2,2',3,4,4',5'-hexachlorobiphenyl	5-MeO-PCB 138	hexa	390.9	346.8

Table S1 (continued)

Source	Congener	Abbreviation	Homlog	Precursor	Product
WellMixC	4-methoxy-2,2',3,4',5,5'-hexachlorobiphenyl	4-MeO-PCB 146	hexa	390.9	346.8
WellMixA	3,3'-dimethoxy-2,2',4,4',6,6'-hexachlorobiphenyl	3,3'-diMeO-PCB 155	hexa, di MeO	420.9	376.7
WellMixXG	4'-methoxy-2,3,3',4,5,5'-hexachlorobiphenyl	4'-MeO-PCB 159	hexa	390.9	346.8
WellMixI	4-methoxy-2,3,3',4',5,5'-hexachlorobiphenyl	4-MeO-PCB 162	hexa	390.9	346.8
WellMixF	4-methoxy-2,3,3',4',5,6-hexachlorobiphenyl	4-MeO-PCB 163	hexa	390.9	346.8
WellMixH	4'-methoxy-2,2',3,3',4,5,5'-heptachlorobiphenyl	4'-MeO-PCB 172	hepta	425.3	382.8
WellMixF	4-methoxy-2,2',3,3',4',5,6-hexachlorobiphenyl	4-MeO-PCB 177	hepta	425.3	382.8
WellMixXB	4-methoxy-2,2',3,3',5,5',6-hexachlorobiphenyl	4-MeO-PCB 178	hepta	425.3	382.8
WellMixG	3'-methoxy-2,2',3,4,4',5,5'-heptachlorobiphenyl	3'-MeO-PCB 180	hepta	425.3	382.8
WellMixC	3'-methoxy-2,2',3,4,4',5,6'-heptachlorobiphenyl	3'-MeO-PCB 182	hepta	425.3	382.8
WellMixD	3'-methoxy-2,2',3,4,4',5',6-hexachlorobiphenyl	3'-MeO-PCB 183	hepta	425.3	382.8
AccuStd	5-methoxy-2,2',3,4,4',5'6-hexachlorobiphenyl	5-MeO-PCB 183	hepta	425.3	382.8
WellMixA	3'-methoxy 2,2',3,4,4',6,6'-heptachlorobiphenyl	3'-MeO-PCB 184	hepta	425.3	382.8
WellMixE	4-methoxy-2,2',3,4',5,5',6-hexachlorobiphenyl	4-MeO-PCB187	hepta	425.3	382.8
WellMixI	4-methoxy-2,3,3',4',5,5',6-hexachlorobiphenyl	4-MeO-PCB193	hepta	425.3	382.8
WellMixD	4'-methoxy-2,2',3,3',4,5,5',6-octachlorobiphenyl	4'-MeO-PCB198	octa	459.8	416.8
WellMixE	4'-methoxy-2,2',3,3',4,5,5',6'-octachlorobiphenyl	4'-MeO-PCB199	octa	459.8	416.8
WellMixF	4'-methoxy-2,2',3,3',4,5,6,6'-octachlorobiphenyl	4'-MeO-PCB200	octa	459.8	416.8
WellMixXB	4'-methoxy-2,2',3,3',4,5',6,6'-octachlorobiphenyl	4'-MeO-PCB201	octa	459.8	416.8
WellMixA	4-methoxy-2,2',3,3',5,5',6,6'-octachlorobiphenyl	4-MeO-PCB202	octa	459.8	416.8
WellMixXG	4,4'-dimethoxy-2,2',3,3',5,5',6,6'-octachlorobiphenyl	4,4'-diMeO-PCB202	octa, di MeO	489.8	446.7
WellMixC	3'-methoxy-2,2',3,4,4',5,5',6-octachlorobiphenyl	3'-MeO-PCB203	octa	459.8	416.8
WellMixC	4'-methoxy 2,2',3,3',4,5,5',6,6'-nonachlorobiphenyl	4'-MeO-PCB208	nona	494.2	450.7

Table S2. OH-PCB congeners and their abbreviations.

Congener	Abbreviation	Congener	Abbreviation
4-hydroxy-2-chlorobiphenyl	4-OH-PCB 1	4'-hydroxy-2,3,3',4,5'-pentachlorobiphenyl	4'-OH-PCB 108
4-hydroxy-3-chlorobiphenyl	4-OH-PCB 2	2'-hydroxy-2,3,4,4',5-pentachlorobiphenyl	2'-OH-PCB 114
6-hydroxy-3-chlorobiphenyl	6-OH-PCB 2	3-hydroxy-2,3',4,4',5-pentachlorobiphenyl	3-OH-PCB 118
4'-hydroxy-4-chlorobiphenyl	4'-OH-PCB 3	4'-hydroxy-2,3',4,5,5'-pentachlorobiphenyl	4'-OH-PCB 120
2'-hydroxy-2,3-dichlorobiphenyl	2'-OH-PCB 5	4'-hydroxy-3,3',4,5,5'-pentachlorobiphenyl	4'-OH-PCB 127
3'-hydroxy-2,5-dichlorobiphenyl	3'-OH-PCB 9	4'-hydroxy-2,2',3,3',4,5'-hexachlorobiphenyl	4'-OH-PCB 130
4'-hydroxy-2,5-dichlorobiphenyl	4'-OH-PCB 9	4-hydroxy-2,2',3,3',5,6-hexachlorobiphenyl	4-OH-PCB 134
2'-hydroxy-3,4-dichlorobiphenyl	2'-OH-PCB 12	3'-hydroxy-2,2',3,4,4',5'-hexachlorobiphenyl	3'-OH-PCB 138
4-hydroxy-3,5-dichlorobiphenyl	4-OH-PCB 14	5-hydroxy-2,2',3,4,4',5'-hexachlorobiphenyl	5-OH-PCB 138
4'-hydroxy-2,2',5-trichlorobiphenyl	4'-OH-PCB 18	4-hydroxy-2,2',3,4',5,5'-hexachlorobiphenyl	4-OH-PCB 146
4'-hydroxy-2,3',5-trichlorobiphenyl	4'-OH-PCB 26	3,3'-dihydroxy-2,2',4,4',6,6'-hexachlorobiphenyl	3,3'-diOH-PCB 155
6'-hydroxy-2,3',5-trichlorobiphenyl	6'-OH-PCB 26	4'-hydroxy-2,3,3',4,5,5'-hexachlorobiphenyl	4'-OH-PCB 159
2'-hydroxy-2,4,6-trichlorobiphenyl	2'-OH-PCB 30	4-hydroxy-2,3,3',4',5,5'-hexachlorobiphenyl	4-OH-PCB 162
3'-hydroxy-2,4,6-trichlorobiphenyl	3'-OH-PCB 30	4-hydroxy-2,3,3',4',5,6-hexachlorobiphenyl	4-OH-PCB 163
4'-hydroxy-2,4,6-trichlorobiphenyl	4'-OH-PCB 30	4'-hydroxy-2,2',3,3',4,5,5'-heptachlorobiphenyl	4'-OH-PCB 172
3-hydroxy-2,2',6,6'-tetrachlorobiphenyl	3-OH-PCB 54	4-hydroxy-2,2',3,3',4',5,6-heptachlorobiphenyl	4-OH-PCB 177
2'-hydroxy-2,3,4,5-tetrachlorobiphenyl	2'-OH-PCB 61	4-hydroxy-2,2',3,3',5,5',6-heptachlorobiphenyl	4-OH-PCB 178
3'-hydroxy-2,3,4,5-tetrachlorobiphenyl	3'-OH-PCB 61	3'-hydroxy-2,2',3,4,4',5,5'-heptachlorobiphenyl	3'-OH-PCB 180
4'-hydroxy-2,3,4,5-tetrachlorobiphenyl	4'-OH-PCB 61	3'-hydroxy-2,2',3,4,4',5,6'-heptachlorobiphenyl	3'-OH-PCB 182
2'-hydroxy-2,3,5,6-tetrachlorobiphenyl	2'-OH-PCB 65	3'-hydroxy-2,2',3,4,4',5',6-heptachlorobiphenyl	3'-OH-PCB 183
3'-hydroxy-2,3,5,6-tetrachlorobiphenyl	3'-OH-PCB 65	5-hydroxy-2,2',3,4,4',5',6-heptachlorobiphenyl	5-OH-PCB 183
4'-hydroxy-2,3',4,6-tetrachlorobiphenyl	4'-OH-PCB 69	3'-hydroxy-2,2',3,4,4',6,6'-heptachlorobiphenyl	3'-OH-PCB 184
6'-hydroxy-2,3',4,6-tetrachlorobiphenyl	6'-OH-PCB 69	4-hydroxy-2,2',3,4',5,5',6-heptachlorobiphenyl	4-OH-PCB 187
4'-hydroxy-2,3',5,5'-tetrachlorobiphenyl	4'-OH-PCB 72	4-hydroxy-2,3,3',4',5,5',6-heptachlorobiphenyl	4-OH-PCB 193
4'-hydroxy-3,3',4,5'-tetrachlorobiphenyl	4'-OH-PCB 79	4'-hydroxy-2,2',3,3',4,5,5',6-octachlorobiphenyl	4'-OH-PCB 198
6'-hydroxy-2,2',3,3',5-pentachlorobiphenyl	6'-OH-PCB 83	4'-hydroxy-2,2',3,3',4,5,5',6'-octachlorobiphenyl	4'-OH-PCB 199
4'-hydroxy-2,2',3,4,5-pentachlorobiphenyl	4'-OH-PCB 86	4'-hydroxy-2,2',3,3',4,5,6,6'-octachlorobiphenyl	4'-OH-PCB 200
4'-hydroxy-2,2',3,5,6-pentachlorobiphenyl	4'-OH-PCB 93	4'-hydroxy-2,2',3,3',4,5',6,6'-octachlorobiphenyl	4'-OH-PCB 201
4'-hydroxy-2,2',3',4,5-pentachlorobiphenyl	4'-OH-PCB 97	4-hydroxy-2,2',3,3',5,5',6,6'-octachlorobiphenyl	4-OH-PCB 202
4'-hydroxy-2,2',4,5,5'-pentachlorobiphenyl	4'-OH-PCB 101	4,4'-dihydroxy-2,2',3,3',5,5',6,6'-octachlorobiphenyl	4,4'-diOH-PCB 202
6'-hydroxy-2,2',4,5,5'-pentachlorobiphenyl	6'-OH-PCB 101	3'-hydroxy-2,2',3,4,4',5,5',6-octachlorobiphenyl	3'-OH-PCB 203
6'-hydroxy-2,3,3',4,5-pentachlorobiphenyl	6'-OH-PCB 106	4'-hydroxy-2,2',3,3',4,5,5',6,6'-nonachlorobiphenyl	4'-OH-PCB 208
4-hydroxy-2,3,3',4',5-pentachlorobiphenyl	4-OH-PCB 107		

Table S3. Limit of Quantification (LOQ) for each OH-PCB congener in sediment in units of nanograms per sample.

Congener	LOQ	Congener	LOQ
4-OH-PCB 1	0.36	3-OH-PCB 118	0.032
6-OH-PCB 2	0.0026	4'-OH-PCB 120	0.16
2'-OH-PCB 5	0.63	4'-OH-PCB 127	0.87
4'-OH-PCB 9 + 4-OH-PCB 14	0.26	4'-OH-PCB 130	0.28
2'-OH-PCB 12	0.00094	4-OH-PCB 134	0.039
4'-OH-PCB 18	0.2	3'-OH-PCB 138	0.068
4'-OH-PCB 26	0.047	5-OH-PCB 138	0.029
6'-OH-PCB 26	0.00062	4-OH-PCB 146	0.35
2'-OH-PCB 30	0.00034	3,3'-diOH-PCB 155	0.0050
3'-OH-PCB 30	0.026	4-OH-PCB 162	0.17
4'-OH-PCB 30	0.056	4-OH-PCB 163	0.036
3-OH-PCB 54	0.0051	4'-OH-PCB 172	0.011
2'-OH-PCB 61	0.0046	4-OH-PCB 177	0.0038
3'-OH-PCB 61	0.15	4-OH-PCB 178	0.0087
2'-OH-PCB 65 + 6'-OH-PCB 69	0.00012	3'-OH-PCB 180	0.014
3'-OH-PCB 65	0.33	3'-OH-PCB 182	0.023
4'-OH-PCB 69	0.029	3'-OH-PCB 183	0.0032
4'-OH-PCB 72	0.030	5-OH-PCB 183 + 4-OH-PCB 187	0.0055
4'-OH-PCB 79	0.028	3'-OH-PCB 184	0.012
6'-OH-PCB 83	0.00034	4-OH-PCB 193	0.0021
4'-OH-PCB 86	0.046	4'-OH-PCB 198 + 4'-OH-PCB 200 + 3'-OH-PCB 203	0.0032
4'-OH-PCB 93	0.20	4'-OH-PCB 199	0.0011
4'-OH-PCB 97	0.016	4'-OH-PCB 201	0.0022
4'-OH-PCB 101	0.011	4-OH-PCB 202	0.0013
6'-OH-PCB 101	0.00064	4,4'-diOH-PCB 202	0.0049
6'-OH-PCB 106 + 2'-OH-PCB 114	0.0017	4'-OH-PCB 208	0.0037

Table S4. Frequency of detection (Det), minimum (Min), maximum (Max), median (Med), average (Ave), and standard deviation (Stdev) of the individual and sum OH-PCBs detected in sediment (n = 20) from Indiana Harbor and Ship Canal, East Chicago, IN. OH-PCBs are reported as nanograms per gram dry weight. Frequency of detection is reported as percent.

Congener	Det	Min	Max	Med	Ave	Stdev
4-OH-PCB 1	0	<LOQ	<LOQ	<LOQ	<LOQ	0.00
6-OH-PCB 2	100	0.03	3.79	0.85	1.14	1.04
2'-OH-PCB 5	10	<LOQ	1.32	<LOQ	0.10	0.33
4'-OH-PCB 9 + 4-OH-PCB 14	15	<LOQ	5.55	<LOQ	0.31	1.24
2'-OH-PCB 12	15	<LOQ	0.17	<LOQ	0.01	0.04
4'-OH-PCB 18	85	<LOQ	3.09	0.66	0.80	0.75
4'-OH-PCB 26	55	<LOQ	0.84	0.05	0.16	0.24
6'-OH-PCB 26	100	0.01	0.78	0.19	0.26	0.22
2'-OH-PCB 30	5	<LOQ	<LOQ	<LOQ	<LOQ	0.00
3'-OH-PCB 30	10	<LOQ	0.05	<LOQ	<LOQ	0.01
4'-OH-PCB 30	5	<LOQ	0.23	<LOQ	0.01	0.05
3-OH-PCB 54	35	<LOQ	0.05	<LOQ	0.01	0.01
2'-OH-PCB 61	50	<LOQ	0.79	0.01	0.13	0.23
3'-OH-PCB 61	0	<LOQ	<LOQ	<LOQ	<LOQ	0.00
2'-OH-PCB 65 + 6'-OH-PCB 69	15	<LOQ	0.01	<LOQ	<LOQ	0.00
3'-OH-PCB 65	95	<LOQ	10.24	3.08	3.79	2.91
4'-OH-PCB 69	85	<LOQ	0.86	0.12	0.21	0.23
4'-OH-PCB 72	30	<LOQ	0.21	<LOQ	0.03	0.06
4'-OH-PCB 79	30	<LOQ	0.03	<LOQ	0.01	0.01
6'-OH-PCB 83	20	<LOQ	0.05	<LOQ	<LOQ	0.01
4'-OH-PCB 86	30	<LOQ	0.29	<LOQ	0.04	0.08
4'-OH-PCB 93	50	<LOQ	0.44	0.06	0.16	0.18
4'-OH-PCB 97	90	<LOQ	0.30	0.12	0.13	0.11
4'-OH-PCB 101	95	<LOQ	0.31	0.10	0.12	0.09
6'-OH-PCB 101	40	<LOQ	0.02	<LOQ	<LOQ	0.01
6'-OH-PCB 106 + 2'-OH-PCB 114	0	<LOQ	<LOQ	<LOQ	<LOQ	0.00
3-OH-PCB 118	10	<LOQ	0.18	<LOQ	0.01	0.05
4'-OH-PCB 120	35	<LOQ	0.14	<LOQ	0.04	0.05
4'-OH-PCB 127	25	<LOQ	1.07	<LOQ	0.17	0.34
4'-OH-PCB 130	0	<LOQ	<LOQ	<LOQ	<LOQ	0.00
4-OH-PCB 134	0	<LOQ	<LOQ	<LOQ	<LOQ	0.00
3'-OH-PCB 138	10	<LOQ	0.06	<LOQ	0.01	0.02
5-OH-PCB 138	50	<LOQ	0.04	0.01	0.01	0.01
4-OH-PCB 146	0	<LOQ	<LOQ	<LOQ	<LOQ	0.00
3,3'-diOH-PCB 155	0	<LOQ	<LOQ	<LOQ	<LOQ	0.00
4-OH-PCB 162	10	<LOQ	0.19	<LOQ	0.01	0.05
4-OH-PCB 163	0	<LOQ	<LOQ	<LOQ	<LOQ	0.00
4'-OH-PCB 172	0	<LOQ	<LOQ	<LOQ	<LOQ	0.00
4-OH-PCB 177	5	<LOQ	0.01	<LOQ	<LOQ	0.00
4-OH-PCB 178	10	<LOQ	0.01	<LOQ	<LOQ	0.00

Table S4 (continued)

Abbreviation	Det	Min	Max	Med	Ave	Stdev
3'-OH-PCB 180	0	<LOQ	<LOQ	<LOQ	<LOQ	0.00
3'-OH-PCB 182	0	<LOQ	<LOQ	<LOQ	<LOQ	0.00
3'-OH-PCB 183	0	<LOQ	<LOQ	<LOQ	<LOQ	0.00
5-OH-PCB 183 + 4-OH-PCB 187	10	<LOQ	0.03	<LOQ	<LOQ	0.01
3'-OH-PCB 184	0	<LOQ	<LOQ	<LOQ	<LOQ	0.00
4-OH-PCB 193	0	<LOQ	<LOQ	<LOQ	<LOQ	0.00
4'-OH-PCB 198 + 4'-OH-PCB 200 + 3'-OH-PCB 203	30	<LOQ	0.01	<LOQ	<LOQ	0.00
4'-OH-PCB 199	25	<LOQ	0.01	<LOQ	<LOQ	0.00
4'-OH-PCB 201	0	<LOQ	<LOQ	<LOQ	<LOQ	0.00
4-OH-PCB 202	0	<LOQ	<LOQ	<LOQ	<LOQ	0.00
4,4'-diOH-PCB 202	0	<LOQ	<LOQ	<LOQ	<LOQ	0.00
4'-OH-PCB 208	10	<LOQ	<LOQ	<LOQ	<LOQ	0.00
Σ OH-PCB ₅₈	100	0.19	26	6.8	7.7	6.2

Table S5. Congener distribution as percent of Σ OH-PCB₆₄ for 5 Aroclors as percent. Values for Aroclors 1221 and 1248 are the average and (standard deviation) of 3 replicates.

Congener	1016	1221	1242	1248	1254
4-OH-PCB 1	0.75	14 (8.9)	0	0.18 (0.16)	0.026
4-OH-PCB 2	0	0	0	1.2 (2.0)	0
6-OH-PCB 2	0.32	5.6 (3.8)	0.69	3.0 (0.03)	0.017
4'-OH-PCB 3	0	0	0	0	0
2'-OH-PCB 5	0	0	0	0	0
3'-OH-PCB 9	0	0	0	0	0.12
4'-OH-PCB 9 + 4-OH-PCB 14	1.5	5.3 (5.6)	0	0.73 (0.26)	0.51
2'-OH-PCB 12	71	0	0	0	0.99
4'-OH-PCB 18	0	2.4 (2.1)	4.1	1.7 (0.17)	0.94
4'-OH-PCB 26	3.4	8.9 (7.2)	6.1	6.4 (0.27)	8.8
6'-OH-PCB 26	0	7.5 (4.4)	5.9	1.2 (0.12)	3.7
2'-OH-PCB 30	0	0	0	0	0
3'-OH-PCB 30	0	0	0	0	0
4'-OH-PCB 30	10	0.42 (0.72)	0	0.17 (0.086)	0
3-OH-PCB 54	2.8	0	0	0	0.15
2'-OH-PCB 61	0	0	0	0	0
3'-OH-PCB 61	0	0	0	0	0
4'-OH-PCB 61	0	0	0	1.3 (0.24)	0.82
2'-OH-PCB 65 + 6'-OH-PCB 69	0.22	0	0	1.1 (0.077)	1.5
3'-OH-PCB 65	7.6	48 (8.8)	69	50 (1.6)	42
4'-OH-PCB 69	0.82	2.0 (1.1)	6.5	4.7 (0.41)	2.9
4'-OH-PCB 72	0.98	0	0	0.13 (0.23)	0
4'-OH-PCB 79	0	0	1.1	0	0
6'-OH-PCB 83	0.003	0	0	0.1 (0.038)	1.7
4'-OH-PCB 86	0	0	0	0.89 (0.77)	0.85
4'-OH-PCB 93	0.23	0	0	2.2 (0.85)	26
4'-OH-PCB 97	0.071	0	0	0.49 (0.075)	4.2
4'-OH-PCB 101	0.036	1.1 (0.1822)	0	0.66 (0.057)	0.81
6'-OH-PCB 101	0	0	0	1.1 (0.23)	0.25
6'-OH-PCB 106 + 2'-OH-PCB 114	0	0	0	0	0
4-OH-PCB 107	0.045	0.18 (0.32)	0.82	0.39 (0.089)	0.38
4'-OH-PCB 108	0	0	0	17 (0.67)	0
3-OH-PCB 118	0	0	0	0.52 (0.22)	0.21
4'-OH-PCB 120	0.092	2.6 (2.9)	5.3	2.0 (0.21)	2
4'-OH-PCB 127	0.13	0	0	2.6 (0.17)	0.59
4'-OH-PCB 130	0.015	0	0	0.067 (0.026)	0.14
4-OH-PCB 134	0.003	0	0	0	0
3'-OH-PCB 138	0	0	0	0.14 (0.033)	0.065
5-OH-PCB 138	0	0.54 (0.4650)	0	0	0.18
4-OH-PCB 146	0.047	1.3 (0.279)	0	0.17 (0.05)	0.43
3,3'-diOH-PCB 155	0	0	0	0	0
4-OH-PCB 162	0	0	0	0	0

Table S5 (continued)

Congener	1016	1221	1242	1248	1254
4-OH-PCB 163	0.0043	0	0	0	0
4'-OH-PCB 172	0	0	0	0	0.009
4-OH-PCB 177	0	0	0	0	0.012
4-OH-PCB 178	0	0	0	0	0.0028
3'-OH-PCB 180	0	0	0	0	0.0049
3'-OH-PCB 182	0	0	0	0	0.097
3'-OH-PCB 183	0	0	0	0	0.013
5-OH-PCB 183 + 4-OH-PCB 187	0	0	0	0	0.047
3'-OH-PCB 184	0	0	0	0	0.023
4-OH-PCB 193	0	0	0	0	0
4'-OH-PCB 198 + 4'-OH-PCB 200 + 3'-OH-PCB 203	0	0	0	0	0
4'-OH-PCB 199	0	0	0	0	0
4'-OH-PCB 201	0	0	0	0	0
4-OH-PCB 202	0	0	0	0	0
4,4'-diOH-PCB 202	0	0	0	0	0
4'-OH-PCB 208	0	0	0	0	0