

Article

Supplementary Materials: Potential Environmental Risk Characteristics of PCB Transformation Products in the Environmental Medium

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Table S1. Estimated statistics of the environmental risk characteristics of PCBs and their transformation products.

Degradation Pathway	Category	Molecular	Phytotoxicity	Change Rate (%)	Estrogen Toxicity	Change Rate (%)	Bioconcentration	Change Rate (%)	Persistence	Change Rate (%)	Migration	Change Rate (%)
Phytodegradation	Molecule	PCB-3	83.95		67.89		2.83		0.18		7.01	
	Degradation products	4 - CBA	66.11	-21.26	60.42	-11.01	4.57	61.26	0.91	421.71	9.27	32.27
	Molecule	PCB-4	73.80		63.98		3.42		0.46		7.41	
	Degradation products	2-CBA	72.80	-1.36	69.30	8.32	4.55	33.06	1.31	183.33	8.49	14.68
	Molecule	PCB-5	79.09		71.67		3.86		0.37		7.44	
	Degradation products	2,3-CBA	77.57	-1.93	69.84	-2.56	5.02	29.99	1.36	268.38	8.69	16.91
	Molecule	PCB-11	83.12		73.81		3.69		0.47		8.19	
	Degradation products	3 - CBA	64.07	-22.92	69.97	-5.20	4.69	27.28	0.73	56.87	8.29	1.22
	Molecule	PCB-31	83.42		70.01		4.16		0.70		7.98	
	Degradation products	2,5-CBA	75.28	-9.76	70.33	0.46	5.08	22.08	1.49	113.34	9.44	18.34
Microbial aerobic degradation	Molecule	PCB-97	76.13		61.49		5.19		1.09		9.40	
	Degradation products	4'-OH-CB97	71.34	-6.30	55.05	-10.48	5.35	3.10	1.13	3.85	8.90	-5.35
	Molecule	PCB-101	72.90		61.50		5.26		1.14		9.31	
	Degradation products	4'-OH-CB101	62.36	-14.46	59.60	-3.08	5.70	8.21	1.11	-2.46	10.24	10.05
	Molecule	PCB-107	84.56		70.57		5.21		1.07		10.16	
	Degradation products	4-OH-CB107	84.60	0.05	67.39	-4.50	5.37	3.05	1.09	2.06	10.34	1.72
	Molecule	PCB-109	67.58		57.75		5.32		1.01		9.65	
	Degradation products	4-OH-CB109	67.77	0.28	59.92	3.76	5.83	9.50	0.95	-6.23	8.01	-17.01
	Molecule	PCB-118	88.52		65.01		5.17		0.96		10.07	
	Degradation products	3-OH-CB118	83.53	-5.64	63.70	-2.01	5.32	2.80	0.84	-13.10	10.11	0.42
	Molecule	PCB-148	70.80		52.26		5.33		1.31		9.61	
	Degradation products	4-OH-CB148	66.70	-5.79	55.92	6.99	5.47	2.53	1.39	6.09	11.39	18.51
	Molecule	PCB-153	66.59		57.17		5.55		1.24		10.03	

Microbial anaerobic degradation	Degradation products	3-OH-CB153	78.53	17.93	59.69	4.40	5.87	5.67	1.39	12.31	9.61	-4.16
	Molecule	PCB-162	86.26		69.84		5.65		1.38		10.65	
	Degradation products	4-OH-CB162	85.20	-1.23	64.24	-8.02	6.00	6.20	1.51	9.67	11.46	7.55
	Molecule	PCB-172	69.30		61.41		6.05		1.58		11.06	
	Degradation products	4'-OH-CB172	66.42	-4.16	55.88	-9.01	5.84	-3.54	1.69	7.04	12.04	8.86
	Molecule	PCB-187	71.07		52.76		5.70		1.56		12.00	
	Degradation products	4-OH-CB187	72.69	2.28	52.85	0.18	5.92	3.72	1.60	2.11	10.80	-10.01
	Molecule	PCB-199	73.26		53.73		5.93		1.74		11.10	
	Degradation products	4'-OH-CB199	85.35	16.50	62.00	15.40	5.61	-5.40	1.08	-37.71	8.92	-19.68
	Molecule	PCB-202	68.26		49.88		5.81		1.81		10.30	
	Degradation products	4-OH-CB202	69.99	2.53	56.65	13.56	5.45	-6.13	2.08	14.67	10.24	-0.66
	Molecule	PCB-90	73.42		60.34		5.12		1.14		9.63	
	Degradation products	PCB-49	71.32	-2.86	61.96	2.68	4.58	-10.56	0.97	-14.96	8.57	-11.03
	Degradation products	PCB-68	90.33	23.02	68.13	12.91	4.73	-7.55	0.86	-24.30	8.74	-9.24
	Molecule	PCB-91	62.97		53.69		5.05		1.05		9.33	
	Degradation products	PCB-51	63.43	0.74	52.78	-1.70	4.55	-9.93	0.90	-14.24	8.44	-9.58
	Molecule	PCB-92	64.06		65.18		5.25		1.16		9.31	
	Degradation products	PCB-52	67.20	4.91	64.52	-1.01	4.71	-10.30	0.99	-14.74	8.54	-8.28
	Degradation products	PCB-72	84.90	32.53	72.84	11.75	4.73	-9.99	0.99	-14.91	8.64	-7.23
	Molecule	PCB-95	65.13		58.46		5.13		1.05		8.99	
	Degradation products	PCB-53	68.36	4.96	66.01	12.92	4.56	-11.08	0.92	-11.75	8.24	-8.32
	Molecule	PCB-99	65.06		56.70		5.13		1.12		9.63	
	Degradation products	PCB-47	65.82	1.16	57.20	0.88	4.63	-9.64	0.83	-25.45	8.89	-7.66
	Molecule	PCB-101	72.90		61.50		5.26		1.14		9.31	
	Degradation products	PCB-49	71.32	-2.17	61.96	0.75	4.58	-13.09	0.97	-15.19	8.57	-7.90
	Molecule	PCB-102	68.29		53.28		5.12		1.11		10.43	
	Degradation products	PCB-51	63.43	-7.11	52.78	-0.93	4.55	-11.09	0.90	-19.04	8.44	-19.10
	Molecule	PCB-130	74.55		62.57		5.48		1.29		10.33	
	Degradation products	PCB-90	73.42	-1.51	60.34	-3.57	5.12	-6.58	1.14	-12.01	9.63	-6.77
	Molecule	PCB-132	66.79		54.86		5.32		1.31		11.04	
	Degradation products	PCB-91	62.97	-5.72	53.69	-2.13	5.05	-4.96	1.05	-19.97	9.33	-15.48
	Molecule	PCB-135	64.86		59.01		5.35		1.33		9.90	
	Degradation products	PCB-94	71.34	9.98	55.61	-5.76	5.08	-5.03	1.09	-17.74	8.94	-9.69
	Molecule	PCB-137	67.12		58.50		5.62		1.29		10.37	
	Degradation products	PCB-90	73.42	9.40	60.34	3.15	5.12	-8.95	1.14	-11.66	9.63	-7.13
	Degradation products	PCB-99	65.06	-3.06	56.70	-3.08	5.13	-8.78	1.12	-13.22	9.63	-7.19
	Molecule	PCB-138	68.89		57.87		5.48		1.24		10.07	

	Degradation products	PCB-99	65.06	-5.56	56.70	-2.02	5.13	-6.43	1.12	-10.22	9.63	-4.42
	Molecule	PCB-146	75.03		60.76		5.55		1.38		10.03	
	Degradation products	PCB-90	73.42	-2.15	60.34	-0.70	5.12	-7.84	1.14	-17.50	9.63	-3.99
	Molecule	PCB-147	65.47		52.28		5.27		1.28		9.95	
	Degradation products	PCB-91	62.97	-3.82	53.69	2.69	5.05	-4.08	1.05	-18.41	9.33	-6.15
	Molecule	PCB-149	68.51		54.16		5.34		1.33		9.71	
	Degradation products	PCB-102	68.29	-0.33	53.28	-1.62	5.12	-4.05	1.11	-16.75	10.43	7.47
	Molecule	PCB-151	67.63		57.03		5.49		1.25		9.65	
	Degradation products	PCB-95	65.13	-3.70	58.46	2.50	5.13	-6.65	1.05	-16.17	8.99	-6.83
	Molecule	PCB-153	66.59		57.17		5.55		1.24		10.03	
	Degradation products	PCB-99	65.06	-2.29	56.70	-0.83	5.13	-7.67	1.12	-9.64	9.63	-3.99
	Molecule	PCB-154	67.69		50.53		5.36		1.23		9.59	
	Degradation products	PCB-100	62.78	-7.27	50.01	-1.03	5.02	-6.36	1.01	-18.00	8.91	-7.09
	Molecule	PCB-170	73.37		58.64		5.96		1.55		11.47	
	Degradation products	PCB-130	74.55	1.61	62.57	6.70	5.48	-8.17	1.29	-16.76	10.33	-9.91
	Degradation products	PCB-137	67.12	-8.52	58.50	-0.24	5.62	-5.77	1.29	-17.09	10.37	-9.56
	Degradation products	PCB-138	68.89	-6.10	57.87	-1.33	5.48	-8.13	1.24	-19.86	10.07	-12.19
	Molecule	PCB-174	70.36		55.18		5.57		1.54		10.60	
	Degradation products	PCB-149	68.51	-2.63	54.16	-1.85	5.34	-4.24	1.33	-13.80	9.71	-8.38
	Molecule	PCB-180	68.69		57.95		6.04		1.53		10.77	
	Degradation products	PCB-153	66.59	-3.06	57.17	-1.34	5.55	-8.10	1.24	-19.12	10.03	-6.92
	Degradation products	PCB-146	75.03	9.24	60.76	4.85	5.55	-8.11	1.38	-9.82	10.03	-6.87
	Molecule	PCB-183	71.55		50.91		5.75		1.55		10.35	
	Degradation products	PCB-154	67.69	-5.38	50.53	-0.73	5.36	-6.71	1.23	-20.72	9.59	-7.36
	Molecule	PCB-187	71.07		52.76		5.70		1.56		12.00	
	Degradation products	PCB-149	68.51	-3.60	54.16	2.65	5.34	-6.45	1.33	-14.90	9.71	-19.09
	Molecule	PCB-49	71.32		61.96		4.58		0.97		8.57	
Biometabolism	Degradation products	3'-MeSO ₂ -CB49	67.66	-5.14	56.88	-8.19	5.46	19.39	0.91	-5.69	10.24	19.44
	Molecule	PCB-64	64.29		57.25		4.78		0.81		8.69	
	Degradation products	4'-MeSO ₂ -CB64	62.72	-2.44	52.25	-8.74	5.27	10.23	1.15	42.10	9.61	10.50
	Molecule	PCB-70	86.77		69.27		4.77		0.96		9.13	
	Degradation products	3'-MeSO ₂ -CB70	78.98	-8.97	66.08	-4.61	5.57	16.77	1.18	22.72	10.99	20.42
	Molecule	PCB-110	68.63		61.74		5.12		1.08		9.84	
	Degradation products	3'-MeSO ₂ -CB110	67.57	-1.56	62.03	0.48	4.98	-2.75	1.17	8.45	9.56	-2.92

Photodegradation	Molecule	PCB-149	68.51		53.15		5.34		1.33		9.71	
	Degradation products	4-MeSO ₂ -CB149	81.80	19.40	54.16	1.89	5.34	0.13	1.63	22.09	10.56	8.82
	Molecule	PCB-174	70.36		56.80		5.57		1.54		10.60	
	Degradation products	4-MeSO ₂ -CB174	72.89	3.60	55.18	-2.86	5.32	-4.45	1.72	11.66	11.12	4.95
	Molecule	PCB-47	65.82		57.20		4.63		0.83		8.89	
	Degradation products	PCB-15	89.55	36.06	65.04	13.72	3.59	-22.50	0.33	-60.70	7.87	-11.43
	Molecule	PCB-40	73.33		65.30		4.56		0.90		9.17	
	Degradation products	PCB-11	83.12	13.35	73.81	13.03	3.69	-19.16	0.47	-48.11	8.19	-10.68
	Molecule	PCB-101	72.90		61.50		5.26		1.14		9.31	
	Degradation products	PCB-70	86.77	19.01	69.27	12.63	4.64	-11.85	0.96	-15.36	9.13	-1.89
	Molecule	PCB-171	70.28		49.26		5.73		1.53		10.72	
	Degradation products	PCB-35	86.14	22.56	69.104	0.28	4.41	-22.93	0.62	-59.57	8.99	-16.20