

SUPPLEMENTARY MATERIAL TO
Environmental behavioral controls of polychlorinated biphenyls: Prediction of the soil sorption coefficient (K_{oc}) using multiple linear regression

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TABLE S-I. List of studied compounds: PCB code, Formulae, observed and prediction values of $\log K_{oc}$.

N°	Compounds	Formulae	$\log K_{oc}$ exp	$\log K_{oc}$ pred
1	PCB-000	C ₁₂ H ₁₀	4.2	4.0244
2	PCB-006	C ₁₂ H ₈ Cl ₂	4.83	4.8731
3	PCB-007	C ₁₂ H ₈ Cl ₂	4.83	4.8719
4	PCB-013	C ₁₂ H ₈ Cl ₂	4.9	4.8944
5	PCB-014	C ₁₂ H ₈ Cl ₂	4.9	4.9257
6*	PCB-017	C ₁₂ H ₇ Cl ₃	5.2	5.2793
7*	PCB-018	C ₁₂ H ₇ Cl ₃	5.2	5.2789
8	PCB-019	C ₁₂ H ₇ Cl ₃	5.28	5.3011
9	PCB-020	C ₁₂ H ₇ Cl ₃	5.23	5.2662
10	PCB-021	C ₁₂ H ₇ Cl ₃	5.19	5.2195
11*	PCB-022	C ₁₂ H ₇ Cl ₃	5.24	5.2511
12	PCB-023	C ₁₂ H ₇ Cl ₃	5.23	5.2823
13	PCB-024	C ₁₂ H ₇ Cl ₃	5.16	5.2409
14*	PCB-025	C ₁₂ H ₇ Cl ₃	5.31	5.316
15*	PCB-026	C ₁₂ H ₇ Cl ₃	5.31	5.3154
16	PCB-027	C ₁₂ H ₇ Cl ₃	5.31	5.2809
17	PCB-029	C ₁₂ H ₇ Cl ₃	5.26	5.2789
18	PCB-031	C ₁₂ H ₇ Cl ₃	5.31	5.2996
19*	PCB-032	C ₁₂ H ₇ Cl ₃	5.23	5.2655
20	PCB-033	C ₁₂ H ₇ Cl ₃	5.31	5.2695
21	PCB-034	C ₁₂ H ₇ Cl ₃	5.31	5.3316
22	PCB-035	C ₁₂ H ₇ Cl ₃	5.33	5.3036

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N°	Compounds	Formulae	log K_{oc} exp	log K_{oc} pred
23	PCB-036	C ₁₂ H ₇ Cl ₃	5.37	5.3677
24	PCB-037	C ₁₂ H ₇ Cl ₃	5.33	5.2874
25	PCB-038	C ₁₂ H ₇ Cl ₃	5.28	5.2775
26	PCB-039	C ₁₂ H ₇ Cl ₃	5.38	5.3522
27	PCB-040	C ₁₂ H ₆ Cl ₄	5.57	5.6343
28*	PCB-041	C ₁₂ H ₆ Cl ₄	5.59	5.6773
29*	PCB-042	C ₁₂ H ₆ Cl ₄	5.64	5.6773
30*	PCB-043	C ₁₂ H ₆ Cl ₄	5.64	5.6922
31	PCB-044	C ₁₂ H ₆ Cl ₄	5.64	5.6762
32	PCB-046	C ₁₂ H ₆ Cl ₄	5.68	5.7182
33*	PCB-047	C ₁₂ H ₆ Cl ₄	5.72	5.722
34*	PCB-048	C ₁₂ H ₆ Cl ₄	5.66	5.6931
35*	PCB-049	C ₁₂ H ₆ Cl ₄	5.71	5.7215
36	PCB-050	C ₁₂ H ₆ Cl ₄	5.76	5.7606
37*	PCB-051	C ₁₂ H ₆ Cl ₄	5.76	5.7443
38	PCB-052	C ₁₂ H ₆ Cl ₄	5.83	5.7213
39	PCB-053	C ₁₂ H ₆ Cl ₄	5.76	5.7415
40	PCB-054	C ₁₂ H ₆ Cl ₄	5.63	5.6795
41	PCB-055	C ₁₂ H ₆ Cl ₄	5.66	5.6624
42*	PCB-056	C ₁₂ H ₆ Cl ₄	5.66	5.6613
43	PCB-057	C ₁₂ H ₆ Cl ₄	5.71	5.7238
44*	PCB-058	C ₁₂ H ₆ Cl ₄	5.71	5.7229
45	PCB-059	C ₁₂ H ₆ Cl ₄	5.64	5.6829
46	PCB-060	C ₁₂ H ₆ Cl ₄	5.67	5.6462
47	PCB-061	C ₁₂ H ₆ Cl ₄	5.61	5.6373
48*	PCB-062	C ₁₂ H ₆ Cl ₄	5.59	5.6523
49	PCB-063	C ₁₂ H ₆ Cl ₄	5.71	5.7092
50	PCB-064	C ₁₂ H ₆ Cl ₄	5.64	5.6677
51	PCB-065	C ₁₂ H ₆ Cl ₄	5.57	5.6631
52	PCB-066	C ₁₂ H ₆ Cl ₄	5.74	5.7107
53	PCB-068	C ₁₂ H ₆ Cl ₄	5.79	5.7736
54	PCB-069	C ₁₂ H ₆ Cl ₄	5.71	5.7393
55	PCB-070	C ₁₂ H ₆ Cl ₄	5.73	5.7106
56*	PCB-071	C ₁₂ H ₆ Cl ₄	5.66	5.6783
57	PCB-072	C ₁₂ H ₆ Cl ₄	5.78	5.7733
58	PCB-073	C ₁₂ H ₆ Cl ₄	5.71	5.738
59*	PCB-074	C ₁₂ H ₆ Cl ₄	5.74	5.7105
60	PCB-075	C ₁₂ H ₆ Cl ₄	5.72	5.7239
61*	PCB-076	C ₁₂ H ₆ Cl ₄	5.68	5.6875
62	PCB-077	C ₁₂ H ₆ Cl ₄	5.75	5.6967
63*	PCB-078	C ₁₂ H ₆ Cl ₄	5.75	5.7198
64	PCB-079	C ₁₂ H ₆ Cl ₄	5.8	5.7612
65	PCB-080	C ₁₂ H ₆ Cl ₄	5.85	5.8256
66	PCB-081	C ₁₂ H ₆ Cl ₄	5.76	5.7034
67	PCB-082	C ₁₂ H ₅ Cl ₅	6	6.0294
68	PCB-083	C ₁₂ H ₅ Cl ₅	6.04	6.0914
69*	PCB-084	C ₁₂ H ₅ Cl ₅	6.09	6.134

N°	Compounds	Formulae	log K_{oc} exp	log K_{oc} pred
70	PCB-085	C ₁₂ H ₅ Cl ₅	6.07	6.0715
71	PCB-086	C ₁₂ H ₅ Cl ₅	6.02	6.0489
72	PCB-087	C ₁₂ H ₅ Cl ₅	6.07	6.0704
73	PCB-088	C ₁₂ H ₅ Cl ₅	6.11	6.1232
74	PCB-089	C ₁₂ H ₅ Cl ₅	6.11	6.1068
75	PCB-090	C ₁₂ H ₅ Cl ₅	6.12	6.1353
76*	PCB-091	C ₁₂ H ₅ Cl ₅	6.11	6.1598
77	PCB-092	C ₁₂ H ₅ Cl ₅	6.11	6.1345
78*	PCB-093	C ₁₂ H ₅ Cl ₅	6.09	6.1494
79	PCB-094	C ₁₂ H ₅ Cl ₅	6.16	6.1741
80*	PCB-095	C ₁₂ H ₅ Cl ₅	5.55	6.157
81	PCB-096	C ₁₂ H ₅ Cl ₅	6.13	6.0979
82*	PCB-097	C ₁₂ H ₅ Cl ₅	6.07	6.0905
83	PCB-098	C ₁₂ H ₅ Cl ₅	6.16	6.1778
84*	PCB-099	C ₁₂ H ₅ Cl ₅	6.14	6.1358
85	PCB-100	C ₁₂ H ₅ Cl ₅	6.24	6.2037
86*	PCB-102	C ₁₂ H ₅ Cl ₅	6.19	6.1629
87	PCB-103	C ₁₂ H ₅ Cl ₅	6.24	6.2011
88	PCB-104	C ₁₂ H ₅ Cl ₅	6.2	6.1384
89	PCB-105	C ₁₂ H ₅ Cl ₅	6.09	6.0569
90	PCB-106	C ₁₂ H ₅ Cl ₅	6.09	6.0802
91*	PCB-107	C ₁₂ H ₅ Cl ₅	6.14	6.1192
92*	PCB-108	C ₁₂ H ₅ Cl ₅	6.14	6.1182
93*	PCB-109	C ₁₂ H ₅ Cl ₅	6.07	6.0942
94*	PCB-110	C ₁₂ H ₅ Cl ₅	6.06	6.0807
95	PCB-111	C ₁₂ H ₅ Cl ₅	6.19	6.1804
96	PCB-112	C ₁₂ H ₅ Cl ₅	6.04	6.1035
97*	PCB-113	C ₁₂ H ₅ Cl ₅	6.11	6.14
98	PCB-114	C ₁₂ H ₅ Cl ₅	6.09	6.0643
99	PCB-115	C ₁₂ H ₅ Cl ₅	6.07	6.0788
100	PCB-116	C ₁₂ H ₅ Cl ₅	5.94	6.013
101*	PCB-117	C ₁₂ H ₅ Cl ₅	6.05	6.0892
102*	PCB-118	C ₁₂ H ₅ Cl ₅	6.16	6.1218
103	PCB-119	C ₁₂ H ₅ Cl ₅	6.16	6.1359
104	PCB-120	C ₁₂ H ₅ Cl ₅	6.32	6.1851
105	PCB-121	C ₁₂ H ₅ Cl ₅	6.19	6.1965
106*	PCB-122	C ₁₂ H ₅ Cl ₅	6.14	6.0779
107	PCB-123	C ₁₂ H ₅ Cl ₅	6.16	6.1289
108	PCB-124	C ₁₂ H ₅ Cl ₅	6.16	6.1287
109*	PCB-125	C ₁₂ H ₅ Cl ₅	6.09	6.0973
110	PCB-126	C ₁₂ H ₅ Cl ₅	6.18	6.1124
111	PCB-127	C ₁₂ H ₅ Cl ₅	6.22	6.1775
112	PCB-129	C ₁₂ H ₄ Cl ₆	6.42	6.449
113*	PCB-130	C ₁₂ H ₄ Cl ₆	6.47	6.4864
114	PCB-131	C ₁₂ H ₄ Cl ₆	6.51	6.5407
115	PCB-132	C ₁₂ H ₄ Cl ₆	6.52	6.5225
116	PCB-133	C ₁₂ H ₄ Cl ₆	6.52	6.5487

N°	Compounds	Formulae	log K_{oc} exp	log K_{oc} pred
117	PCB-134	C ₁₂ H ₄ Cl ₆	6.49	6.5676
118	PCB-135	C ₁₂ H ₄ Cl ₆	6.57	6.5899
119	PCB-136	C ₁₂ H ₄ Cl ₆	6.53	6.5171
120	PCB-137	C ₁₂ H ₄ Cl ₆	6.49	6.4918
121	PCB-139	C ₁₂ H ₄ Cl ₆	6.59	6.5664
122*	PCB-140	C ₁₂ H ₄ Cl ₆	6.59	6.5661
123*	PCB-141	C ₁₂ H ₄ Cl ₆	6.49	6.4905
124	PCB-142	C ₁₂ H ₄ Cl ₆	6.46	6.4912
125*	PCB-143	C ₁₂ H ₄ Cl ₆	6.54	6.5293
126	PCB-144	C ₁₂ H ₄ Cl ₆	6.59	6.5635
127	PCB-145	C ₁₂ H ₄ Cl ₆	6.56	6.5
128	PCB-146	C ₁₂ H ₄ Cl ₆	6.54	6.5486
129*	PCB-147	C ₁₂ H ₄ Cl ₆	6.57	6.5927
130	PCB-148	C ₁₂ H ₄ Cl ₆	6.64	6.6334
131*	PCB-149	C ₁₂ H ₄ Cl ₆	6.59	6.5781
132	PCB-150	C ₁₂ H ₄ Cl ₆	6.61	6.5564
133*	PCB-151	C ₁₂ H ₄ Cl ₆	6.56	6.5895
134	PCB-152	C ₁₂ H ₄ Cl ₆	6.53	6.5329
135*	PCB-154	C ₁₂ H ₄ Cl ₆	6.66	6.6221
136	PCB-155	C ₁₂ H ₄ Cl ₆	6.08	6.5966
137*	PCB-156	C ₁₂ H ₄ Cl ₆	6.51	6.4746
138	PCB-157	C ₁₂ H ₄ Cl ₆	6.51	6.4737
139*	PCB-158	C ₁₂ H ₄ Cl ₆	6.49	6.4914
140*	PCB-159	C ₁₂ H ₄ Cl ₆	6.56	6.5361
141	PCB-160	C ₁₂ H ₄ Cl ₆	6.42	6.4548
142	PCB-161	C ₁₂ H ₄ Cl ₆	6.56	6.5507
143	PCB-162	C ₁₂ H ₄ Cl ₆	6.56	6.5362
144*	PCB-163	C ₁₂ H ₄ Cl ₆	6.47	6.5004
145	PCB-164	C ₁₂ H ₄ Cl ₆	6.49	6.4988
146*	PCB-165	C ₁₂ H ₄ Cl ₆	6.52	6.5606
147	PCB-166	C ₁₂ H ₄ Cl ₆	6.42	6.4396
148	PCB-167	C ₁₂ H ₄ Cl ₆	6.58	6.5407
149	PCB-168	C ₁₂ H ₄ Cl ₆	6.56	6.5556
150	PCB-169	C ₁₂ H ₄ Cl ₆	6.6	6.5293
151	PCB-170	C ₁₂ H ₃ Cl ₇	6.85	6.844
152	PCB-171	C ₁₂ H ₃ Cl ₇	6.94	6.9289
153	PCB-172	C ₁₂ H ₃ Cl ₇	6.89	6.9062
154	PCB-173	C ₁₂ H ₃ Cl ₇	6.87	6.9084
155	PCB-174	C ₁₂ H ₃ Cl ₇	6.94	6.9448
156*	PCB-175	C ₁₂ H ₃ Cl ₇	6.99	6.9962
157	PCB-176	C ₁₂ H ₃ Cl ₇	6.96	6.9185
158*	PCB-177	C ₁₂ H ₃ Cl ₇	6.92	6.9554
159	PCB-178	C ₁₂ H ₃ Cl ₇	6.97	7.0238
160	PCB-179	C ₁₂ H ₃ Cl ₇	6.94	6.9551
161	PCB-180	C ₁₂ H ₃ Cl ₇	6.92	6.9051
162	PCB-181	C ₁₂ H ₃ Cl ₇	6.94	6.9341
163	PCB-182	C ₁₂ H ₃ Cl ₇	7.02	6.9888

N°	Compounds	Formulae	log K_{oc} exp	log K_{oc} pred
164*	PCB-183	C ₁₂ H ₃ Cl ₇	7.02	6.9841
165	PCB-184	C ₁₂ H ₃ Cl ₇	7.03	6.9583
166	PCB-186	C ₁₂ H ₃ Cl ₇	6.91	6.8684
167	PCB-187	C ₁₂ H ₃ Cl ₇	6.99	7.0114
168	PCB-188	C ₁₂ H ₃ Cl ₇	7.01	6.9908
169	PCB-189	C ₁₂ H ₃ Cl ₇	6.94	6.892
170	PCB-190	C ₁₂ H ₃ Cl ₇	6.84	6.8519
171*	PCB-191	C ₁₂ H ₃ Cl ₇	6.92	6.909
172	PCB-192	C ₁₂ H ₃ Cl ₇	6.89	6.9119
173*	PCB-193	C ₁₂ H ₃ Cl ₇	6.89	6.9193
174	PCB-194	C ₁₂ H ₂ Cl ₈	7.3	7.2637
175*	PCB-196	C ₁₂ H ₂ Cl ₈	7.37	7.351
176	PCB-197	C ₁₂ H ₂ Cl ₈	7.39	7.3204
177*	PCB-198	C ₁₂ H ₂ Cl ₈	7.35	7.3641
178	PCB-199	C ₁₂ H ₂ Cl ₈	7.31	7.3781
179	PCB-200	C ₁₂ H ₂ Cl ₈	7.36	7.2913
180	PCB-201	C ₁₂ H ₂ Cl ₈	7.34	7.3563
181	PCB-202	C ₁₂ H ₂ Cl ₈	7.34	7.3938
182	PCB-203	C ₁₂ H ₂ Cl ₈	7.37	7.3527
183	PCB-204	C ₁₂ H ₂ Cl ₈	7.39	7.3261
184	PCB-205	C ₁₂ H ₂ Cl ₈	7.27	7.2711
185	PCB-206	C ₁₂ H ₁ Cl ₉	7.72	7.719
186	PCB-207	C ₁₂ H ₁ Cl ₉	7.74	7.6926
187	PCB-208	C ₁₂ H ₁ Cl ₉	7.72	7.7321
188	PCB-209	C ₁₂ Cl ₁₀	8.09	8.0695

TABLE S-II. Genetic algorithm settings in QSARINS software

GA until	02 (number of the descriptors in the model)
Generation per size	500
Population size	10
Mutation rate	20