

Electronic supplementary information (ESI) for the paper

**QSPR as a support for the EU REACH regulation and rational design of environmentally
safer chemicals: PBT identification from molecular structure**

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pp. 2-6: Table S1

pp. 7-8: Table S2

Table S1. List of the studied 250 chemicals. For each compound reported here are given: ID number, CAS number, experimental (in bold) or predicted log BCF, Log(1/LC50)96h and extrapolated GHLI values (15, 19-21), PC1 scores from PCA-A and PCA-B (PCA-B scores are reported as Experimental (Exp. PBT INDEX) to distinguish them from values predicted by Equation 1), values for the descriptors included in Equation 1, experimental PBT Index values calculated by PCA (PCA-B), values of the PBT Index predicted by Equation 1, hat values for the Applicability Domain of Equation 1 (** = out of the AD), PBT category derived from cut off values proposed in this paper (PBT Index cat.) and from US EPA PBT Profiler (PBT US EPA cat.). The last two columns of Table 1 were used in this paper to compare the PBT Index and the US EPA PBT Profiler.

ID	CAS	Log BCF	Log (1/LC50)	GHLI	PC1 Scores PCA_A	PC1 Scores PCA_B (Exp PBT Index)	nBM	nX	MAXDP	nHDon	PBT Index	PBT Index Pred	AD Eq.1	PBT Index cat.	PBT US EPA cat. ^a
1	000050-29-3	4.84	6.35	2.764	--	3.85	12	5	2.002	0	3.85	4.24	0.058	3	3
2	000050-32-8	--	--	--	--	--	24	0	0.309	0	--	3.7	0.127**	3	3
3	000053-70-3	--	--	--	--	--	26	0	0.333	0	--	4.13	0.15**	3	3
4	000055-21-0	1.6	2.26	-1.515	--	-1.09	7	0	3.423	2	-1.09	-0.97	0.044	1	1
5	000056-23-5	--	--	--	--	--	0	4	0.715	0	--	1.1	0.04	2	2
6	000056-38-2	1.99	4.69	-0.477	--	0.53	9	0	3.504	0	0.53	0.23	0.022	2	2
7	000056-55-3	--	--	--	--	--	21	0	0.299	0	--	3.06	0.096**	3	3
8	000057-74-9	--	--	--	--	--	1	8	2.508	0	--	3.78	0.127**	3	3
9	000058-89-9	2.84	4.33	3.091	--	2.02	0	6	1.77	0	2.02	2.32	0.072	3	2
10	000060-29-7	0.73	2.15	-0.477	--	-1.25	0	0	1.333	0	-1.25	-1.54	0.021	1	1
11	000060-35-5	-0.29	1.32	-1.515	--	-2.5	1	0	2.222	2	-2.5	-2.17	0.048	1	1
12	000060-57-1	3.87	4.67	2.857	--	2.64	1	6	2.713	0	2.64	2.46	0.072	3	3
13	000062-53-3	0.41	2.95	-1.415	-1.86	-1.38	6	0	1.358	2	-1.38	-1.03	0.05	1	1
14	000062-55-5	-0.31	2.01	-1.515	--	-2.2	1	0	0.843	2	-2.2	-2.07	0.06	1	1
15	000062-75-9	-0.31	1.26	-1.038	--	-2.37	1	0	2.181	0	-2.37	-1.39	0.017	1	1
16	000063-25-2	1.22	4.36	-0.573	-0.17	-0.05	12	0	4.092	1	-0.05	0.45	0.035	2	2
17	000064-17-5	--	--	--	--	--	0	0	1.569	1	--	-1.95	0.022	1	1
18	000064-18-6	--	--	--	--	--	1	0	1.361	1	--	-1.72	0.021	1	1
19	000064-19-7	-0.21	1.75	-1.598	--	-2.29	1	0	2	1	-2.29	-1.76	0.018	1	1
20	000065-85-0	1.69	3.35	-1.598	--	-0.59	7	0	3.201	1	-0.59	-0.56	0.015	1	1
21	000067-56-1	--	--	--	--	--	0	0	1	1	--	-1.91	0.027	1	1
22	000067-63-0	-0.49	0.84	-2.297	--	-3.08	0	0	2.056	1	-3.08	-1.98	0.02	1	1
23	000067-64-1	-0.17	0.91	-0.558	--	-2.29	1	0	2.444	0	-2.29	-1.41	0.018	1	1
24	000067-66-3	1.11	3.23	2.204	-0.08	0.33	0	3	0.694	0	0.33	0.45	0.03	2	1
25	000067-72-1	2.92	5.22	2.682	2.54	2.32	0	6	1.033	0	2.32	2.37	0.074	3	2
26	000069-72-7	1.43	3.63	-1.598	--	-0.6	7	0	3.262	2	-0.6	-0.95	0.044	1	1
27	000071-23-8	-0.47	1.12	-2.297	--	-2.94	0	0	1.875	1	-2.94	-1.97	0.021	1	1
28	000071-36-3	-0.02	1.63	-2.297	--	-2.48	0	0	2.066	1	-2.48	-1.99	0.02	1	1
29	000071-41-0	0.37	2.27	-2.297	--	-1.99	0	0	2.197	1	-1.99	-2	0.02	1	1
30	000071-43-2	0.64	3.5	-0.817	-1.18	-0.81	6	0	0	0	-0.81	-0.15	0.026	1	1
31	000072-43-5	3.1	6.21	-0.118	--	1.91	12	3	2.073	0	1.91	2.93	0.03	3	3
32	000072-55-9	4.71	6.42	3.776	--	4.16	13	4	1.86	0	4.16	3.82	0.046	3	3
33	000074-97-5	0.6	3.51	0.944	--	-0.23	0	2	0.804	0	-0.23	-0.21	0.023	2	1
34	000075-01-4	--	--	--	--	--	1	1	0.651	0	--	-0.63	0.02	1	1
35	000075-04-7	--	--	--	--	--	0	0	0.847	2	--	-2.28	0.062	1	1
36	000075-07-0	--	--	--	--	--	1	0	1.806	0	--	-1.36	0.017	1	1
37	000075-09-2	1.36	2.41	2.204	-0.4	0.1	0	2	0.653	0	0.1	-0.19	0.024	2	1
38	000075-27-4	--	--	--	--	--	0	3	0.846	0	--	0.44	0.028	2	1
39	000075-65-0	0.7	1.06	-1.037	-2.68	-1.93	0	0	2.521	1	-1.93	-2.02	0.02	1	1
40	000075-99-0	0.86	2.87	0.904	--	-0.4	1	2	2.757	1	-0.4	-0.52	0.021	2	1
41	000076-01-7	1.83	4.43	2.682	1.29	1.4	0	5	1.024	0	1.4	1.73	0.054	2	2
42	000078-83-1	-0.08	1.71	-2.297	--	-2.48	0	0	2.144	1	-2.48	-1.99	0.02	1	1

43	000078-87-5	0.85	2.95	1.969	-0.51	-0.01	0	2	1.219	0	-0.01	-0.24	0.02	2	1
44	000078-93-3	0.21	1.35	-1.695	--	-2.28	1	0	2.813	0	-2.28	-1.44	0.019	1	1
45	000079-01-6	1.59	3.47	0.701	-0.06	0.18	1	3	0.846	0	0.18	0.66	0.026	2	1
46	000079-10-7	0.28	2.29	-1.842	--	-1.88	2	0	2.25	1	-1.88	-1.57	0.015	1	1
47	000079-11-8	-0.07	2.54	-0.095	--	-1.37	1	1	2.236	1	-1.37	-1.13	0.016	1	1
48	000079-20-9	--	--	--	--	--	1	0	2.59	0	--	-1.42	0.018	1	1
49	000079-34-5	1.11	3.92	2.682	0.48	0.8	0	4	1.003	0	0.8	1.08	0.038	2	1
50	000080-62-6	0.86	2.57	-1.842	--	-1.45	2	0	3.19	0	-1.45	-1.25	0.02	1	1
51	000084-66-2	2.07	3.85	-0.339	0.18	0.25	8	0	4.544	0	0.25	-0.06	0.036	2	1
52	000084-74-2	2.22	5.45	-0.573	1.18	0.96	8	0	4.945	0	0.96	-0.09	0.044	2	1
53	000085-01-8	3.4	5.43	1.164	--	2.15	16	0	0.178	0	2.15	1.99	0.059	3	2
54	000085-68-7	1.21	6.23	-0.573	--	0.77	14	0	5.243	0	0.77	1.18	0.069	2	1
55	000086-30-6	1.33	3.91	-1.038	--	-0.35	13	0	3.782	0	-0.35	1.07	0.038	2	2
56	000086-73-7	3.23	5.35	1.164	--	2.03	12	0	0.218	0	2.03	1.13	0.037	3	1
57	000087-62-7	2	3.72	-1.07	--	-0.09	6	0	1.682	2	-0.09	-1.05	0.047	2	2
58	000088-06-2	2.43	4.61	0.36	1.11	1.01	6	3	3.008	1	1.01	1.19	0.026	2	2
59	000088-72-2	1.26	3.47	-0.445	--	-0.38	8	0	3.227	0	-0.38	0.04	0.018	2	2
60	000088-75-5	1.6	2.94	-0.9	-0.87	-0.59	8	0	3.067	1	-0.59	-0.34	0.015	1	1
61	000088-99-3	1.43	3.94	-1.598	--	-0.47	8	0	3.463	2	-0.47	-0.75	0.046	2	1
62	000090-05-1	1.73	3.3	-1.842	--	-0.68	6	0	2.986	1	-0.68	-0.76	0.013	1	1
63	000090-12-0	1.73	4.8	-0.118	--	0.57	11	0	0.157	0	0.57	0.91	0.034	2	1
64	000091-20-3	1.93	4.32	-0.118	0.44	0.46	11	0	0.12	0	0.46	0.92	0.035	2	2
65	000091-22-5	0.58	3.84	-0.573	--	-0.61	11	0	1.181	0	-0.61	0.84	0.023	1	1
66	000091-59-8	2.57	4.03	-1.415	--	0.23	11	0	1.624	2	0.23	0.03	0.058	2	2
67	000092-52-4	2.64	4.84	-0.573	--	0.91	12	0	0.12	0	0.91	1.13	0.038	2	1
68	000092-87-5	--	--	--	--	--	12	0	1.609	4	--	-0.53	0.221**	1	2
69	000094-75-7	2.23	4.98	-1.144	--	0.56	7	2	3.157	1	0.56	0.74	0.019	2	1
70	000094-82-6	2.17	5.37	-1.271	--	0.66	7	2	3.223	1	0.66	0.74	0.019	2	2
71	000095-15-8	2.43	4.42	0.701	--	1.04	10	0	0.139	0	1.04	0.7	0.031	2	1
72	000095-47-6	1.24	3.81	0.222	-0.25	-0.01	6	0	0.12	0	-0.01	-0.16	0.025	2	1
73	000095-48-7	1.03	3.89	-3.134	-1.38	-1.22	6	0	2.919	1	-1.22	-0.76	0.013	1	1
74	000095-50-1	2.48	4.19	1.969	1.39	1.39	6	2	1.466	0	1.39	1.04	0.011	2	2
75	000095-51-2	0.95	4.35	-0.573	-0.37	-0.19	6	1	1.473	2	-0.19	-0.39	0.05	2	2
76	000095-53-4	1.88	3.25	-2.794	--	-0.94	6	0	1.52	2	-0.94	-1.04	0.048	1	1
77	000095-63-6	2.08	4.19	0.222	0.57	0.6	6	0	0.204	0	0.6	-0.17	0.024	2	2
78	000095-93-2	--	--	--	--	--	6	0	0.241	0	--	-0.17	0.023	2	2
79	000095-94-3	3.76	5.8	2.544	3.44	2.97	6	4	1.5	0	2.97	2.33	0.028	3	2
80	000095-95-4	2.73	5	-0.36	--	1.1	6	3	2.95	1	1.1	1.19	0.026	2	2
81	000096-09-3	1.82	3.56	-0.817	--	-0.17	6	0	1.595	0	-0.17	-0.27	0.012	2	1
82	000096-18-4	1.11	3.41	1.969	-0.05	0.33	0	3	1.275	0	0.33	0.41	0.026	2	2
83	000096-22-0	0.57	1.75	-1.271	--	-1.78	1	0	3.181	0	-1.78	-1.47	0.022	1	1
84	000098-82-8	1.55	4.13	0.222	--	0.29	6	0	0.204	0	0.29	-0.17	0.024	2	1
85	000098-86-2	2.34	2.87	-0.793	--	-0.19	7	0	3.645	0	-0.19	-0.21	0.021	2	1
86	000098-95-3	0.67	3.02	0.296	-1.11	-0.63	8	0	3.006	0	-0.63	0.06	0.016	1	1
87	000099-99-0	0.9	3.61	-0.445	--	-0.5	8	0	3.118	0	-0.5	0.05	0.017	2	2
88	000100-02-7	0.71	3.49	-0.9	-1.16	-0.81	8	0	3.036	1	-0.81	-0.33	0.015	1	1
89	000100-41-4	1.19	4.01	0.222	-0.17	0.05	6	0	0.162	0	0.05	-0.16	0.024	2	1
90	000100-42-5	1.13	4.41	-1.07	-0.36	-0.24	7	0	0.631	0	-0.24	0.02	0.019	2	1
91	000100-51-6	1.97	3.14	-2.297	--	-0.77	6	0	2.538	1	-0.77	-0.73	0.012	1	1
92	000100-66-3	1.66	3.35	-0.477	--	-0.23	6	0	1.414	0	-0.23	-0.26	0.012	2	1
93	000101-84-8	2.5	4.63	-0.477	0.92	0.78	12	0	2.078	0	0.78	0.99	0.024	2	1
94	000103-65-1	--	--	--	--	--	6	0	0.201	0	--	-0.17	0.023	2	1
95	000103-82-2	2.1	3.55	-1.598	--	-0.29	7	0	3.169	1	-0.29	-0.56	0.015	2	1
96	000105-67-9	2.18	3.87	-1.842	-0.19	-0.19	6	0	3.044	1	-0.19	-0.77	0.013	2	1

97	000106-42-3	1.27	4.08	0.222	-0.07	0.12	6	0	0.12	0	0.12	-0.16	0.025	2	1
98	000106-46-7	2.62	4.56	1.969	1.71	1.63	6	2	1.442	0	1.63	1.04	0.011	3	2
99	000106-47-8	0.84	3.61	-1.768	-1.26	-0.98	6	1	1.445	2	-0.98	-0.38	0.051	1	2
100	000106-99-0	--	--	--	--	--	2	0	0.361	0	--	-1.04	0.024	1	1
101	000107-02-8	0.17	6.52	-2.794	--	-0.39	2	0	2.056	0	-0.39	-1.17	0.015	2	1
102	000107-06-2	0.3	2.86	2.204	-0.87	-0.25	0	2	0.943	0	-0.25	-0.22	0.021	2	1
103	000107-12-0	0.01	1.56	0.48	--	-1.56	1	0	1.625	0	-1.56	-1.35	0.017	1	1
104	000107-13-1	1.68	2.48	-1.271	--	-0.87	2	0	1.507	0	-0.87	-1.13	0.015	1	1
105	000107-18-6	-0.03	5.26	-2.297	--	-0.89	1	0	1.757	1	-0.89	-1.75	0.018	1	1
106	000107-21-1	--	--	--	--	--	0	0	1.625	2	--	-2.34	0.054	1	1
107	000107-30-2	-0.93	2.31	-0.477	--	-2.05	0	1	0.853	0	-2.05	-0.86	0.021	1	1
108	000107-31-3	--	--	--	--	--	1	0	1.951	0	--	-1.37	0.017	1	1
109	000107-87-9	0.57	2.51	-1.271	--	-1.44	1	0	3.044	0	-1.44	-1.46	0.021	1	1
110	000107-92-6	0.24	2.59	-1.598	--	-1.69	1	0	2.599	1	-1.69	-1.81	0.017	1	1
111	000108-05-4	0.84	2.43	-1.598	--	-1.44	2	0	2.75	0	-1.44	-1.22	0.017	1	1
112	000108-10-1	0.86	2.28	-1.271	--	-1.39	1	0	3.254	0	-1.39	-1.47	0.023	1	1
113	000108-38-3	1.27	3.82	0.222	-0.22	0.01	6	0	0.167	0	0.01	-0.16	0.024	2	1
114	000108-60-1	1.08	3.27	-0.477	--	-0.57	0	2	1.785	0	-0.57	-0.28	0.018	1	2
115	000108-67-8	2.27	4.61	0.222	--	0.88	6	0	0.188	0	0.88	-0.17	0.024	2	2
116	000108-70-3	3.38	5.07	1.969	--	2.25	6	3	1.47	0	2.25	1.69	0.017	3	2
117	000108-86-1	1.7	4.01	1.725	--	0.82	6	1	0.561	0	0.82	0.46	0.016	2	2
118	000108-87-2	--	--	--	--	--	0	0	0.36	0	--	-1.47	0.029	1	1
119	000108-88-3	1.12	3.41	0.222	-0.58	-0.25	6	0	0.083	0	-0.25	-0.16	0.025	2	1
120	000108-89-4	1.42	2.36	0.944	--	-0.31	6	0	0.846	0	-0.31	-0.21	0.016	2	1
121	000108-90-7	1.85	3.82	1.725	0.65	0.82	6	1	1.429	0	0.82	0.39	0.009	2	1
122	000108-91-8	--	--	--	--	--	0	0	1.635	2	--	-2.34	0.054	1	1
123	000108-93-0	0.89	2.15	-2.297	--	-1.77	0	0	2.909	1	-1.77	-2.05	0.021	1	1
124	000108-94-1	1.07	2.2	-1.271	--	-1.31	1	0	3.463	0	-1.31	-1.49	0.025	1	1
125	000108-95-2	1.24	3.46	-1.842	-1.1	-0.86	6	0	2.632	1	-0.86	-0.73	0.012	1	1
126	000108-99-6	1.4	2.81	0.944	--	-0.13	6	0	0.884	0	-0.13	-0.22	0.016	2	1
127	000109-60-4	0.55	3.23	-1.598	--	-1.24	1	0	2.98	0	-1.24	-1.45	0.021	1	1
128	000109-66-0	--	--	--	--	--	0	0	0.212	0	--	-1.46	0.031	1	1
129	000109-67-1	--	--	--	--	--	1	0	0.55	0	--	-1.27	0.024	1	1
130	000109-73-9	-0.11	2.44	-2.541	--	-2.26	0	0	1.139	2	-2.26	-2.3	0.059	1	1
131	000109-94-4	--	--	--	--	--	1	0	2.183	0	--	-1.39	0.017	1	1
132	000109-99-9	0.14	1.52	-0.817	--	-1.95	0	0	1.444	0	-1.95	-1.55	0.021	1	1
133	000110-00-9	0.7	3.05	-0.817	-1.41	-0.98	5	0	1.083	0	-0.98	-0.45	0.014	1	1
134	000110-02-1	0.95	3.18	-0.201	--	-0.58	5	0	0.042	0	-0.58	-0.37	0.026	1	1
135	000110-43-0	1.15	2.94	-1.271	--	-0.95	1	0	3.319	0	-0.95	-1.48	0.024	1	1
136	000110-54-3	--	--	--	--	--	0	0	0.232	0	--	-1.46	0.031	1	1
137	000110-75-8	0.44	2.99	-0.477	--	-1.03	1	1	1.115	0	-1.03	-0.66	0.016	1	1
138	000110-82-7	--	--	--	--	--	0	0	0	0	--	-1.44	0.034	1	1
139	000110-83-8	--	--	--	--	--	1	0	0.267	0	--	-1.25	0.028	1	1
140	000110-86-1	0.99	2.9	0.944	--	-0.3	6	0	0.785	0	-0.3	-0.21	0.017	2	1
141	000111-27-3	0.7	3.02	-2.297	--	-1.49	0	0	2.293	1	-1.49	-2	0.02	1	1
142	000111-42-2	--	--	--	--	--	0	0	2.149	3	--	-2.76	0.111**	1	1
143	000111-43-3	0.4	3.21	-0.477	--	-0.95	0	0	1.632	0	-0.95	-1.57	0.02	1	1
144	000111-44-4	1.04	3.31	-0.477	--	-0.57	0	2	1.368	0	-0.57	-0.25	0.019	1	1
145	000111-65-9	--	--	--	--	--	0	0	0.256	0	--	-1.46	0.031	1	3
146	000111-66-0	--	--	--	--	--	1	0	0.658	0	--	-1.28	0.023	1	1
147	000111-87-5	--	--	--	--	--	0	0	2.423	1	--	-2.01	0.02	1	1
148	000111-91-1	0.62	3.85	-0.477	--	-0.55	0	2	1.372	0	-0.55	-0.25	0.019	1	1
149	000112-40-3	--	--	--	--	--	0	0	0.279	0	--	-1.46	0.03	1	2
150	000114-26-1	1.47	4.38	-0.73	--	0.04	7	0	4.03	1	0.04	-0.62	0.022	2	1

151	000115-10-6	--	--	--	--	--	0	0	0.75	0	--	-1.5	0.025	1	1
152	000116-06-3	0.38	2.83	0.322	--	-0.86	2	0	3.532	1	-0.86	-1.66	0.02	1	1
153	000118-74-1	--	--	--	--	--	6	6	1.558	0	--	3.63	0.065	3	3
154	000118-90-1	2.11	3.7	-1.598	--	-0.22	7	0	3.422	1	-0.22	-0.58	0.016	2	1
155	000118-91-2	1	3.93	0.701	--	0.08	7	1	3.337	1	0.08	0.08	0.015	2	1
156	000119-61-9	1.08	4.09	-0.793	-0.5	-0.31	13	0	4.846	0	-0.31	0.99	0.056	2	1
157	000120-12-7	3.26	5.49	1.164	--	2.1	16	0	0.241	0	2.1	1.99	0.058	3	2
158	000120-80-9	1.34	4.08	-1.842	--	-0.54	6	0	2.669	2	-0.54	-1.12	0.042	1	1
159	000120-82-1	3.32	4.78	1.969	2.33	2.1	6	3	1.486	0	2.1	1.69	0.017	3	2
160	000120-83-2	1.53	4.32	-0.9	-0.08	-0.01	6	2	2.853	1	-0.01	0.55	0.016	2	2
161	000121-14-2	0.96	3.88	-0.445	-0.61	-0.35	10	0	3.38	0	-0.35	0.46	0.023	2	2
162	000121-69-7	0.9	3.19	-1.07	-1.26	-0.9	6	0	0.083	0	-0.9	-0.16	0.025	1	2
163	000121-75-5	1.52	4.37	-2.173	-0.45	-0.42	3	0	4.802	0	-0.42	-1.16	0.042	2	1
164	000122-34-9	--	--	--	--	--	6	1	1.568	2	--	-0.39	0.049	2	2
165	000122-39-4	2.18	4.65	-1.07	0.52	0.42	12	0	0.804	1	0.42	0.7	0.036	2	2
166	000123-38-6	-0.17	2.1	-2.794	--	-2.52	1	0	2.174	0	-2.52	-1.39	0.017	1	1
167	000123-72-8	0.2	3.69	-2.794	--	-1.63	1	0	2.405	0	-1.63	-1.41	0.018	1	1
168	000123-86-4	0.71	3.81	-1.598	--	-0.9	1	0	3.096	0	-0.9	-1.46	0.022	1	1
169	000123-91-1	-0.3	0.93	-0.573	-3.32	-2.36	0	0	1.444	0	-2.36	-1.55	0.021	1	1
170	000124-18-5	--	--	--	--	--	0	0	0.27	0	--	-1.46	0.03	1	1
171	000124-40-3	--	--	--	--	--	0	0	0.25	1	--	-1.85	0.036	1	1
172	000126-99-8	1.13	2.96	0.466	--	-0.36	2	1	1.039	0	-0.36	-0.44	0.014	2	1
173	000129-00-0	--	--	--	--	--	19	0	0.212	0	--	2.63	0.08	3	3
174	000131-11-3	1.76	3.97	-0.339	--	0.14	8	0	4.225	0	0.14	-0.04	0.03	2	1
175	000132-64-9	3.34	4.9	0.126	--	1.54	15	0	2.152	0	1.54	1.63	0.038	3	1
176	000134-32-7	1.4	3.94	-1.415	--	-0.42	11	0	1.756	2	-0.42	0.02	0.057	2	2
177	000137-26-8	0.53	3.63	-0.339	--	-0.65	2	0	1.406	0	-0.65	-1.12	0.016	1	1
178	000141-43-5	--	--	--	--	--	0	0	1.75	3	--	-2.74	0.115**	1	1
179	000141-78-6	1.48	2.58	-1.598	-1.38	-1.04	1	0	2.822	0	-1.04	-1.44	0.02	1	1
180	000142-29-0	--	--	--	--	--	1	0	0.236	0	--	-1.25	0.028	1	1
181	000142-62-1	0.76	3.46	-1.598	--	-1.03	1	0	2.874	1	-1.03	-1.83	0.018	1	1
182	000198-55-0	--	--	--	--	--	24	0	0.247	0	--	3.71	0.128**	3	3
183	000206-44-0	--	--	--	--	--	19	0	0.22	0	--	2.63	0.08	3	3
184	000207-08-9	--	--	--	--	--	24	0	0.333	0	--	3.7	0.127**	3	3
185	000218-01-9	--	--	--	--	--	21	0	0.236	0	--	3.06	0.097**	3	3
186	000287-92-3	--	--	--	--	--	0	0	0	0	--	-1.44	0.034	1	1
187	000292-64-8	--	--	--	--	--	0	0	0	0	--	-1.44	0.034	1	1
188	000298-00-0	1.93	4.49	-0.477	--	0.41	9	0	3.412	0	0.41	0.24	0.021	2	2
189	000309-00-2	3.74	4.79	2.359	--	2.45	2	6	2.651	0	2.45	2.68	0.07	3	3
190	000319-86-8	2.57	4.33	3.091	--	1.88	0	6	1.77	0	1.88	2.32	0.072	3	2
191	000330-54-1	1.15	4.22	0.222	-0.07	0.12	7	2	4.247	1	0.12	0.66	0.029	2	2
192	000330-55-2	1.25	4.15	0.222	--	0.15	7	2	4.353	1	0.15	0.65	0.031	2	2
193	000333-41-5	1.85	4.51	1.271	0.93	0.97	7	0	2.185	0	0.97	-0.1	0.012	2	2
194	000462-06-6	1.63	2.87	-0.817	--	-0.57	6	1	3.907	0	-0.57	0.21	0.021	1	1
195	000496-11-7	--	--	--	--	--	6	0	0.238	0	--	-0.17	0.023	2	1
196	000526-73-8	2.29	4.57	0.222	--	0.88	6	0	0.157	0	0.88	-0.16	0.024	2	2
197	000534-52-1	0.46	5.06	0.36	0	0.18	10	0	3.372	1	0.18	0.07	0.022	2	2
198	000541-73-1	2.65	4.26	1.969	1.55	1.52	6	2	1.449	0	1.52	1.04	0.011	3	2
199	000542-88-1	--	--	--	--	--	0	2	0.884	0	--	-0.21	0.022	2	1
200	000581-40-8	--	--	--	--	--	11	0	0.241	0	--	0.91	0.033	2	2
201	000591-50-4	2.14	4.27	1.725	--	1.17	6	1	0.16	0	1.17	0.49	0.021	2	2
202	000591-78-6	0.87	2.37	-1.271	--	-1.34	1	0	3.203	0	-1.34	-1.47	0.022	1	1
203	000591-87-7	0.85	2.65	-1.598	--	-1.34	2	0	2.933	0	-1.34	-1.23	0.018	1	1
204	000591-93-5	--	--	--	--	--	2	0	0.479	0	--	-1.05	0.023	1	1

205	000592-84-7	0.52	3.1	-1.598	--	-1.32	1	0	2.457	0	-1.32	-1.41	0.018	1	1
206	000608-93-5	3.86	6	3.446	3.9	3.41	6	5	1.544	0	3.41	2.98	0.044	3	3
207	000621-64-7	--	--	--	--	--	1	0	2.961	0	--	-1.45	0.02	1	2
208	000625-38-7	0.66	2.48	-1.842	--	-1.6	2	0	2.528	1	-1.6	-1.59	0.015	1	1
209	000628-41-1	--	--	--	--	--	2	0	0.181	0	--	-1.03	0.027	1	1
210	000628-63-7	0.91	3.57	-1.598	--	-0.9	1	0	3.185	0	-0.9	-1.47	0.022	1	1
211	000634-66-2	3.77	5.29	2.544	3.13	2.75	6	4	1.523	0	2.75	2.33	0.028	3	2
212	000634-90-2	3.59	5.75	2.544	--	2.86	6	4	1.516	0	2.86	2.33	0.028	3	2
213	000693-02-7	--	--	--	--	--	1	0	0.965	0	--	-1.3	0.021	1	1
214	000759-94-4	1.26	3.2	-1.162	--	-0.74	1	0	4.412	0	-0.74	-1.56	0.039	1	2
215	001127-76-0	--	--	--	--	--	11	0	0.197	0	--	0.91	0.033	2	1
216	001563-66-2	1.63	5.42	-1.07	--	0.47	7	0	4.154	1	0.47	-0.63	0.024	2	2
217	001582-09-8	--	--	--	--	--	10	3	4.845	0	--	2.3	0.052	3	3
218	001634-04-4	0.18	2.12	-0.477	-2.23	-1.55	0	0	1.438	0	-1.55	-1.55	0.021	1	1
219	001746-01-6	--	--	--	--	--	12	4	2.138	0	--	3.58	0.041	3	3
220	001912-24-9	--	--	--	--	--	6	1	1.616	2	--	-0.4	0.049	2	2
221	001918-00-9	2.24	4.62	-0.233	--	0.72	7	2	3.731	1	0.72	0.7	0.023	2	1
222	002051-24-3	--	--	--	--	--	12	10	2.092	0	--	7.48	0.212**	3	3
223	002051-61-8	3.52	5.07	2.397	--	2.47	12	1	1.784	0	2.47	1.66	0.021	3	2
224	002303-16-4	2.07	3.49	0.549	--	0.39	2	2	4.806	0	0.39	-0.07	0.043	2	2
225	002303-17-5	2.3	3.75	-0.37	--	0.32	2	3	4.875	0	0.32	0.57	0.052	2	2
226	002539-17-5	3.08	5.54	0.36	--	1.76	6	4	3.399	1	1.76	1.81	0.043	3	2
227	003268-87-9	--	--	--	--	--	12	8	2.128	0	--	6.18	0.136**	3	3
228	003424-82-6	4.31	6.25	3.776	--	3.87	13	4	2.056	0	3.87	3.8	0.046	3	3
229	005409-83-6	3.39	6.09	1.399	--	2.52	15	2	2.145	0	2.52	2.93	0.038	3	3
230	007005-72-3	2.92	5.37	-0.477	--	1.32	12	1	2.075	0	1.32	1.64	0.021	2	2
231	007085-19-0	1.89	4.75	-1.162	--	0.28	7	1	3.531	1	0.28	0.06	0.017	2	1
232	008001-35-2	--	--	--	--	--	1	8	2.488	0	--	3.78	0.127**	3	3
233	017804-35-2	--	--	--	--	--	12	0	5.305	2	--	-0.03	0.078	2	1
234	055702-46-0	4.23	6.07	3.68	--	3.72	12	3	2.006	0	3.72	2.94	0.03	3	3
235	076842-07-4	5.47	7.12	4.255	--	5.02	12	5	2.01	0	5.02	4.24	0.058	3	3
236	013029-08-8	3.74	5.5	2.397	--	2.78	12	2	1.961	0	2.78	2.29	0.023	3	3
237	032774-16-6	--	--	--	--	--	12	6	1.86	0	--	4.9	0.079	3	3
238	068194-16-1	--	--	--	--	--	12	7	2.062	0	--	5.53	0.105**	3	3
239	030746-58-8	--	--	--	--	--	12	4	2.14	0	--	3.58	0.041	3	3
240	033820-53-0	--	--	--	--	--	10	0	4.441	0	--	0.38	0.038	2	3
241	033857-26-0	2.54	6.23	1.058	--	2.02	12	2	2.145	0	2.02	2.28	0.023	3	3
242	035822-46-9	--	--	--	--	--	12	7	2.132	0	--	5.53	0.105**	3	3
243	038964-22-6	2.82	6.22	1.058	--	2.16	12	2	2.145	0	2.16	2.28	0.023	3	3
244	039001-02-0	--	--	--	--	--	15	8	2.128	0	--	6.82	0.151**	3	2
245	039227-54-8	2.7	5.65	1.058	--	1.85	12	1	2.149	0	1.85	1.63	0.021	3	3
246	039227-58-2	2.75	6.66	1.058	--	2.32	12	3	2.144	0	2.32	2.93	0.03	3	3
247	039227-61-7	--	--	--	--	--	12	5	2.137	0	--	4.23	0.058	3	3
248	051207-31-9	--	--	--	--	--	15	4	2.138	0	--	4.23	0.056	3	3
249	051218-45-2	2.26	4.56	1.027	--	1.13	7	1	5.188	0	1.13	0.33	0.046	2	2
250	052663-77-1	--	--	--	--	--	12	9	2.085	0	--	6.83	0.171**	3	3

^a To simplify the categorization originally proposed by US EPA PBT Profiler chemicals were assigned to: cat. 3 = three criteria were exceeded, cat 2 = two out three criteria were exceeded, cat. 1 = one or none criterion were exceeded. If one of the properties was not evaluated by the US EPA PBT Profiler, it was accounted as if the criterion for that property was exceeded.

Table S2. PBT screening performed for 45 compounds from DSL list.

ID CAS	CAS	Name ^a	A - PBT Profiler ^b	B - DSL	C - Log HAF	C - Log HAF III	D - PBT Index	A - PBT Profiler	B - DSL	C - Log HAF & HAF III	D - PBT Index	Consensus
1	000050-00-0	formaldehyde	1	DSL 0	-6.22	-4.69	-1.303	non PBT	non PBT	non PBT	non PBT	non PBT
2	000050-32-8	benzo a pyrene	3	DSL I	-2.61	-1.12	3.705	PBT	PBT	PBT	PBT	PBT
3	000053-19-0	o,p'-DDD	3	DSL I	-2.65	-1.23	3.583	PBT	PBT	PBT	PBT	PBT
4	000059-50-7	4-chloro 3-methylphenol	2	DSL I	-3.25	-3.29	-0.104	non PBT	PBT	non PBT	non PBT	non PBT*
5	000062-56-6	thiourea	1	DSL 0	-7.98	-5.99	-2.822	non PBT	non PBT	non PBT	non PBT	non PBT
6	000074-85-1	ethene	1	DSL 0	-11.76	-8.1	-1.229	non PBT	non PBT	non PBT	non PBT	non PBT
7	000074-96-4	bromoethane	1	DSL 0	-8.96	-8.07	-0.824	non PBT	non PBT	non PBT	non PBT	non PBT
8	000075-26-3	2-bromopropane	1	DSL 0	-8.96	-7.59	-0.834	non PBT	non PBT	non PBT	non PBT	non PBT
9	000075-34-3	1,1 dichloroethane	1	DSL 0	-8.64	-7.77	-0.215	non PBT	non PBT	non PBT	non PBT	non PBT
10	000075-35-4	1,1 dichloroethene	1	DSL 0	-9.88	-7.49	0.015	non PBT	non PBT	non PBT	non PBT	non PBT
11	000076-44-8	heptachlor	3	POP	-3.73	-0.47	2.689	PBT	PBT	PBT	PBT	PBT
12	000077-47-4	1,2,3,4,5,5-hexachloro-1,3cyclopentadiene	3	DSL I	-3.44	-1.78	2.766	PBT	PBT	PBT	PBT	PBT
13	000078-40-0	triethylester phosphoric acid	1	DSL 0	-7.64	-7.55	-1.554	non PBT	non PBT	non PBT	non PBT	non PBT
14	000079-06-1	2-propenamide	1	DSL 0	-5	-2.37	-1.971	non PBT	non PBT	non PBT	non PBT	non PBT
15	000079-92-5	Camphene	1	DSL 0	-9.62	-5.45	-1.318	non PBT	non PBT	non PBT	non PBT	non PBT
16	000079-94-7	tetrabromobisphenol A	3	DSL I	-2.96	1.43	2.678	PBT	PBT	PBT	PBT	PBT
17	000080-05-7	Bisphenol A	2	DSL 0	-3.03	-2.84	0.122	non PBT	non PBT	non PBT	non PBT	non PBT
18	000086-74-8	9H-Carbazole	1	DSL I	-3.98	-3.54	1.244	non PBT	PBT	non PBT	non PBT	non PBT*
19	000087-86-5	pentachlorophenol	2	DSL I	-2.78	-1.53	2.47	non PBT	PBT	PBT	PBT	PBT*
20	000087-90-1	1,3,5, trichloro-1,3,5 triazine-2,4,6,(1H, 3H, 5H)-trione	2	DSL I	-2.83	-0.58	0.87	non PBT	PBT	PBT	non PBT	PBT*
21	000094-58-6	1,3 benzodioxole, 5 propyl	2	DSL 0	-6.7	-5.13	-0.283	non PBT	non PBT	non PBT	non PBT	non PBT
22	000095-76-1	3,4-dichloro-benzeneamine	2	DSL I	-2.45	-1.33	0.263	non PBT	PBT	PBT	non PBT	PBT*
23	000096-23-1	1,3-dichloro-2-propanol	1	DSL 0	-7.21	-7.04	-0.712	non PBT	non PBT	non PBT	non PBT	non PBT
24	000104-40-5	4-nonylphenol	2	DSL 0	-3.84	-2.21	-0.773	non PBT	non PBT	PBT	non PBT	non PBT*
25	000106-70-7	hexanoic acyd, methylester	1	DSL 0	-8.14	-7.84	-1.488	non PBT	non PBT	non PBT	non PBT	non PBT
26	000106-93-4	1,2 dibromoethane	1	DSL I	-3.59	-3.6	-0.179	non PBT	PBT	non PBT	non PBT	non PBT*
27	000107-05-1	3-chloro-1-propene	1	DSL 0	-8.13	-5.34	-0.651	non PBT	non PBT	non PBT	non PBT	non PBT
28	000110-12-3	5-methyl-2-hexanone	1	DSL 0	-8.27	-7.44	-1.479	non PBT	non PBT	non PBT	non PBT	non PBT
29	000110-82-7	cyclohexane	1	DSL 0	-9.84	-6.26	-1.444	non PBT	non PBT	non PBT	non PBT	non PBT
30	000115-07-1	1-propene	1	DSL 0	-11.88	-7.68	-1.256	non PBT	non PBT	non PBT	non PBT	non PBT
31	000118-74-1	hexachlorobenzene *	3	POP	-1.46	0.02	3.629	PBT	PBT	PBT	PBT	PBT

32	000124-18-5	decane	1	DSL 0	-9.92	-4.8	-1.464	non PBT	non PBT	non PBT	non PBT	non PBT
33	000129-00-0	pyrene	3	DSL I	-0.2	1.16	2.635	PBT	PBT	PBT	PBT	PBT
34	000132-65-0	Dibenzothiphen	1	DSL I	-3.91	-3.24	1.774	non PBT	PBT	non PBT	PBT	PBT*
35	000271-89-6	benzofuran	1	DSL 0	-7.59	-6.13	0.59	non PBT	non PBT	non PBT	non PBT	non PBT
36	000626-39-1	1,3,5-tribromobenzene	2	DSL I	-4.35	-3.71	1.752	non PBT	PBT	non PBT	PBT	PBT*
37	001582-09-8	trifluralin	3	DSL I	-1.08	0.16	2.297	PBT	PBT	PBT	PBT	PBT
38	001912-24-9	atrazine *	2	DSL I	-0.29	-0.02	-0.396	non PBT	PBT	PBT	non PBT	PBT*
39	002051-24-3	decachlorobiphenyl (PCB 209)	3	POP	-2.7	-1.78	7.479	PBT	PBT	PBT	PBT	PBT
40	002385-85-5	Mirex	3	POP	-2.13	-1.1	6.148	PBT	PBT	PBT	PBT	PBT
41	003268-87-9	octachlorodibenzo- <i>p</i> -dioxin	3	POP	-2.95	-1.78	6.178	PBT	PBT	PBT	PBT	PBT
42	025569-80-6	PCB 6	3	POP	-4.02	-2.61	2.294	PBT	PBT	PBT	PBT	PBT
43	032598-10-0	PCB 66	3	POP	-2.59	-1.25	3.591	PBT	PBT	PBT	PBT	PBT
44	035065-27-1	PCB 153	3	POP	-2.18	-0.9	4.888	PBT	PBT	PBT	PBT	PBT
45	035694-08-7	PCB 194	3	POP	-2.21	-1.18	6.183	PBT	PBT	PBT	PBT	PBT

a: compounds with unhomogeneous screening are marked as (*)

b: 3 = all P, B, and T criteria exceeded; 2 = 2 out of 3 criteria exceeded; 1 = 1 or 0 criteria exceeded. If one of the properties was not evaluated by the model, it was accounted as if the criterion for that property was exceeded .