

**Multi-species QSAR modeling for predicting aquatic toxicity of diverse organic
chemicals for regulatory toxicology**

Supporting information

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Table S1: Toxicity of selected chemical compounds in algae (*P. subcapitata*), daphnia and fish for QSAR modeling

S.No	CAS No.	Chemical name	Algae (EC ₅₀) mg/L	Daphnia (EC ₅₀) mg/L	Fish (LC ₅₀) mg/L
1	50-06-6	Barbituric acid, 5-ethyl-5-phenyl-	>100	>96	-
2	53-70-3	Dibenzo[a,h]anthracene	>0.0013	>0.016	>0.014
3	56-23-5	Carbon tetrachloride	0.46	8.1	7.6
4	57-09-0	N,N,N-trimethyl-1-hexadecanaminium	0.0064	0.016	0.28
5	57-10-3	Palmitic acid	>0.60	>4.8	>6.9
6	57-14-7	N,N-Dimethylhydrazine	3.4	1.3	-
7	57-55-6	Propylene glycol	>1000	>1000	>100
8	58-27-5	Menadione	0.23	0.22	-
9	58-90-2	2,3,4,6-Tetrachlorophenol	2.1	1.4	0.56
10	59-51-8	DL-Methionine	>1000	>1000	>100
11	60-00-4	Ethylenediaminetetraacetic acid	6.0	57	74
12	60-09-3	Aniline, p-(phenylazo)- <p-	2.9	0.46	0.35
13	60-24-2	2-Mercaptoethanol	0.17	0.12	29
14	60-34-4	Methylhydrazine	0.28	0.95	0.38
15	60-80-0	Phenazone	>1000	>1000	>100
16	61-82-5	3-Amino-1,2,4-triazole	65	-	-
17	62-53-3	Aniline	110	0.32	27
18	62-56-6	Thiourea	>100	16	>110
19	63-74-1	Sulphanilamide	23	13	-
20	67-63-0	2-Propanol	>1000	>1000	>100
21	68-11-1	Mercaptoacetic acid	>4.4	36	40
22	68-12-2	Dimethylformamide	>1000	>1000	>100
23	69-72-7	Salicylic acid	65	77	39
24	71-36-3	1-Butanol	>1000	>1000	>100
25	75-05-8	Acetonitrile	>700	>1000	>100
26	75-07-0	Acetaldehyde	26	30	-
27	75-08-1	Ethanethiol	3.0	0.077	2.2
28	75-12-7	Formamide	>1000	-	-
29	75-18-3	Dimethyl sulphide	>540	330	>100
30	75-26-3	2-Bromopropane	>260	23	>67
31	75-27-4	Bromodichloromethane	12	29	28
32	75-34-3	1,1-Dichloroethane	>94	34	-
33	75-35-4	Ethene, 1,1-dichloro-	-	16 ^a	45 ^b
34	75-50-3	Trimethylamine	>100	28	>100
35	75-65-0	2-Methylpropan-2-ol	>110	>110	>120
36	75-98-9	Pivalic acid	66	87	-
37	76-06-2	Trichloronitromethane	0.000078	0.11	0.01
38	76-13-1	1,1,2-Trichloro-1,2,2-trifluoroethane	>4.1	4.3	19
39	77-47-4	Hexachlorocyclopentadiene	-	0.0091 ^a	0.014 ^b
40	77-67-8	Ethosuximide	-	>99 ^a	-
41	77-85-0	2-Hydroxymethyl-2-methyl-1,3-	>1000	>1000	>100
42	78-59-1	3,5,5-Trimethyl-2-cyclohexen-1-one	230	220	>100
43	78-67-1	2,2'-Azobis(2-methylpropanenitrile)	>7.8	>10	>10
44	78-70-6	1,6-Octadiene-3-ol, 3,7-dimethyl-	>34	52	39
45	78-79-5	Isoprene	67	3.2	15

46	78-87-5	1,2-Dichloropropane	140	30	160
47	78-93-3	2-Butanone	>1200	>1000	>100
48	79-01-6	Trichloroethylene	77	11	38
49	79-10-7	Acrylic acid	0.75	47	62
50	79-11-8	Chloroacetic acid	0.16	-	72
51	79-14-1	Glycolic acid	>32	44	78
52	79-19-6	Thiosemicarbazide	19	12	21
53	79-39-0	Methacrylamide	>1000	>1000	>100
54	79-94-7	Tetrabromobisphenol A	9.5	7.9	9.2
55	80-04-6	Hydrogenatedbisphenol A	81	31	19
56	80-05-7	Bisphenol A	4.8	13	8.0
57	80-09-1	Bis(4-hydroxyphenyl)sulfone	65	100	-
58	80-43-3	Di-a-cumyl peroxide	>15	0.26	0.47
59	80-51-3	4,4'-Oxybis(benzenesulfonylhydrazide)	>0.81	2.9	>6.6
60	80-62-6	Methyl methacrylate <2-Propenoic acid,	>86	84	-
61	82-68-8	Pentachloronitrobenzene	>0.91	0.93	0.32
62	83-32-9	Acenaphthene	>0.62	1.3	>2.1
63	84-15-1	o-Terphenyl	>8.3	0.52	0.12
64	84-61-7	Dicyclohexyl phthalate	>2.0	>2.0	>2.0
65	84-65-1	Anthraquinone	>0.035	>0.24	>0.40
66	84-69-5	Diisobutyl phthalate	1.8	6.7	3.0
67	84-74-2	Dibutyl phthalate	2.7	4.8	2.8
68	85-01-8	Phenanthrene	0.64	1.1	1.4
69	85-41-6	Phthalimide	>150	21	100
70	85-44-9	Phthalic anhydride	68	71	>99
71	85-68-7	Butyl benzyl phthalate	-	-	>1.1 ^b
72	86-30-6	N-Nitrosodiphenylamine	>3.1	10	10
73	86-73-7	Fluorene	0.76	0.49	>1.2
74	86-74-8	Carbazole	>0.65	>0.72	>0.82
75	87-59-2	2,3-Dimethylaniline	41	8.9	>94
76	87-61-6	1,2,3-Trichlorobenzene	1.6	0.46	3.2
77	87-62-7	2,6-Dimethylaniline	>100	20	>98
78	87-82-1	Hexabromobenzene	>0.00008	>0.00021	>0.00009
79	87-83-2	2,3,4,5,6-Pentabromotoluene	>0.0073	>0.0073	>0.0073
80	87-86-5	Pentachlorophenol	0.86	0.11	0.19
81	88-05-1	2,4,6-Trimethylaniline	27	12	55
82	88-09-5	Butanoic acid, 2-ethyl-	73	72	85
83	88-18-6	2-tert-Butylphenol	1.3	3.7	3.7
84	88-19-7	o-Toluenesulfonamide	170	210	>100
85	88-44-8	6-Amino-m-toluenesulfonic acid	>10	>10	>10
86	88-60-8	6-tert-Butyl-m-cresol	1.9	3.0	2.7
87	88-74-4	o-Nitroaniline	44	10	42
88	88-75-5	o-Nitrophenol	6.0	28	64
89	88-85-7	Phenol, 2-(1-methylpropyl)-4,6-	1.4	0.4	0.28
90	89-04-3	Trioctyl benzene-1,2,4-tricarboxylate	>25	-	-
91	89-40-7	4-Nitrophthalimide	-	28 ^a	11 ^b
92	89-63-4	4-Chloro-2-nitroaniline	8.5	4.2	17
93	89-64-5	4-Chloro-2-nitrophenol	6.2	7.9	11
94	89-72-5	o-sec-Butylphenol	6.9	4.0	6.0
95	89-83-8	Thymol	14	4.5	4.7
96	90-02-8	2-Hydroxybenzaldehyde	4.8	2.6	1.6

97	90-04-0	o-Anisidine	>30	23	200
98	90-05-1	2-Methoxyphenol	270	29	>100
99	90-12-0	1-Methylnaphthalene	2.8	2.2	5.7
100	90-13-1	1-Chloronaphthalene	>2.2	0.73	1.7
101	90-30-2	1-(N-phenylamino)-naphthalene	0.034	0.26	0.7
102	90-60-8	3,5-Dichlorosalicylaldehyde	-	1.4 ^a	-
103	91-15-6	Phthalonitrile	140	210	23
104	91-17-8	Bicyclo[4.4.0]decane	>0.051	0.23	0.37
105	91-22-5	Quinoline	66	25	67
106	91-23-6	o-Nitroanisole	57	46	47
107	91-53-2	6-Ethoxy-1,2-dihydro-2,2,4-	0.7	0.76	6.7
108	91-57-6	2-Methylnaphthalene	1.9	1.4	1.9
109	91-59-8	β -Naphthylamine	0.5	0.84	3.9
110	91-66-7	N,N-Diethylaniline	2.8	11	26
111	91-76-9	2,4-Diamino-6-phenyl-s-triazine	71	52	-
112	91-94-1	3,3'-Dichlorobenzidine	1.4	1.9	0.51
113	92-06-8	m-Terphenyl	>2.4	0.65	3.1
114	92-52-4	Biphenyl	0.78	1.4	3.9
115	92-69-3	p-Phenylphenol	2.4	3.9	3.4
116	92-70-6	3-Hydroxy-2-naphthoic acid	64	33	>82
117	92-84-2	Phenothiazine	0.74	0.055	>0.96
118	92-88-6	Biphenyl-4,4'-diol	5.7	1.8	13
119	93-15-2	4-Allyl-1,2-dimethoxybenzene	22	38	14
120	93-68-5	o-Acetoacetotoluidide	750	930	>100
121	93-83-4	N,N-Bis(2-hydroxyethyl)oleamide	>55	0.05	1.5
122	95-08-9	2,2'-Ethylenedioxydiethyl bis(2-	>31	28	9.4
123	95-16-9	Benzothiazole	>46	19	39
124	95-31-8	N-(tert-Butyl)-2-	0.095	1.3	1.4
125	95-32-9	2-(4'-Morpholinodithio)benzothiazole	>0.054	0.58	0.49
126	95-33-0	N-Cyclohexyl-2-	0.15	0.79	2.1
127	95-47-6	o-Xylene	0.8	1.1	7.4
128	95-49-8	o-Chlorotoluene	7.8	0.7	7.7
129	95-50-1	o-Dichlorobenzene	>4.2	1.4	3.8
130	95-51-2	o-Chloroaniline	28	2.0	7.3
131	95-53-4	o-Toluidine	120	16	150
132	95-54-5	o-Phenylenediamine	0.82	1.4	4.6
133	95-55-6	o-Aminophenol	0.15	0.57	0.67
134	95-64-7	3,4-Dimethylaniline	8.6	1.1	>98
135	95-70-5	2,5-Diaminotoluene	2.0	0.46	0.19
136	95-75-0	3,4-Dichlorotoluene	1.4	1.4	4.3
137	95-76-1	3,4-Dichloroaniline	6.5	0.55	11
138	95-78-3	2,5-Dimethylaniline	30	18	-
139	95-80-7	2,4-Diaminotoluene	18	15	-
140	95-81-8	2-Chloro-5-methylaniline	4.9	3.6	11
141	95-82-9	2,5-Dichloroaniline	9.6	1.8	2.2
142	95-87-4	2,5-Xylenol	29	5.2	5.7
143	95-95-4	2,4,5-Trichlorophenol	1.5	0.98	1.5
144	96-09-3	Styrene oxide	25	1.9	8.8
145	96-12-8	1,2-Dibromo-3-chloropropane	62	19	39
146	96-23-1	1,3-Dichloro-2-propanol	630	730	>100
147	96-29-7	2-Butanone oxime	16	200	-

148	96-33-3	Methyl acrylate	3.1	2.6	1.4
149	96-76-4	2,4-Di-tert-butylphenol	1.0	0.33	0.68
150	96-96-8	2-Nitro-p-anisidine	12	4.4	41
151	97-00-7	1-Chloro-2,4-dinitrobenzene	0.18	0.66	0.16
152	97-39-2	N,N'-Bis(2-methylphenyl)guanidine	8.6	7.2	19
153	97-88-1	n-Butyl methacrylate	23	25	5.6
154	97-99-4	Tetrahydrofurfuryl alcohol	>100	>92	>100
155	98-08-8	Benzotrifluoride	5.4	3.1	19
156	98-51-1	4-tert-Butyltoluene	4.4	1.5	1.7
157	98-59-9	4-Toluenesulfonyl chloride <p-Toluene	57	72	77
158	98-81-7	alpha-Bromostyrene	-	0.33 ^a	0.15 ^b
159	98-83-9	2-Phenylpropene	4.8	2.6	7.3
160	98-87-3	alpha,alpha-Dichlorotoluene	27	22	23
161	99-04-7	m-Toluic acid	17	75	82
162	99-09-2	Benzenamine, 3-nitro- <m-Nitroaniline>	43	9.1	90
163	99-54-7	3,4-Dichloronitrobenzene	2.5	5.2	4.7
164	99-65-0	Benzene, m-dinitro-	-	35 ^a	12 ^b
165	99-71-8	p-sec-Butylphenol	7.5	3.1	2.6
166	99-76-3	Methyl p-hydroxybenzoate	56	36	60
167	99-82-1	p-Menthane	>2.5	0.12	0.19
168	99-87-6	p-Cymene	5.8	1.9	2.0
169	99-88-7	4-Isopropylaniline	18	1.5	46
170	99-94-5	4-Methylbenzoic acid	74	42	64
171	99-96-7	4-Hydroxybenzoic acid	110	140	93
172	99-99-0	p-Nitrotoluene	10	4.3	37
173	100-01-6	p-Nitroaniline	43	22	85
174	100-14-1	alpha-Chloro-4-nitrotoluene	0.038	1.5	0.61
175	100-21-0	Terephthalic acid	>18	>20	>19
176	100-40-3	4-Vinylcyclohexene	>4.1	1.9	4.6
177	100-43-6	4-Vinylpyridine	4.6	1.2	1.0
178	100-51-6	Benzyl alcohol	770	230	>100
179	100-52-7	Benzaldehyde	32	-	-
180	100-54-9	3-Cyanopyridine	-	41 ^a	-
181	100-55-0	3-Hydroxymethylpyridine	-	680 ^a	930 ^b
182	100-61-8	N-Methylaniline	>20	5.6	58
183	100-63-0	Hydrazine, phenyl-	-	0.016 ^a	0.016 ^b
184	100-64-1	Cyclohexanone oxime	9.8	72	>100
185	100-69-6	2-Vinylpyridine	62	9.5	6.5
186	100-74-3	4-Ethylmorpholine	53~80	>92	-
187	100-97-0	Hexamethylenetetramine	>100	>100	>100
188	101-02-0	Triphenyl phosphite	>16	0.45	>4.3
189	101-14-4	4,4'-Methylenebis(2-chloroaniline)	>0.85	0.92	0.61
190	101-20-2	3,4,4'-Trichlorodiphenylurea	0.048	0.016	>0.031
191	101-77-9	4,4'-Methylenedianiline	12	2.5	21
192	101-80-4	4,4'-Diaminodiphenyl ether	28	0.99	>52
193	101-83-7	Dicyclohexylamine	>19	8.0	12
194	101-84-8	Diphenyl ether	0.58	2.0	1.8
195	101-96-2	1,4-Benzenediamine, N,N'-bis(1-	0.94	0.54	0.37
196	102-06-7	1,3-Diphenylguanidine	7.6	8.1	17
197	102-76-1	Triacetin <triacetyl glycerine>	>940	770	>100
198	102-81-8	2-(Dibutylamino)ethanol	21	-	29

199	103-23-1	Bis(2-ethylhexyl) adipate	>50	>50	>50
200	103-24-2	Dioctyl azelate	>0.013	>0.093	>0.072
201	103-50-4	Dibenzyl ether	4.1	0.77	6.8
202	103-69-5	N-Ethylaniline	33	11	67
203	103-90-2	N-(4-Hydroxyphenyl) acetamide	>460	3.5	-
204	104-51-8	Butylbenzene	1.6	1.0	3.3
205	104-94-9	p-Anisidine	13	4.1	-
206	105-16-8	2-(Diethylamino)ethyl methacrylate	>10	360	-
207	105-53-3	Diethyl malonate	880	190	39
208	105-60-2	Caprolactam	>1000	>1000	>100
209	105-67-9	2,4-Xylenol	9.7	2.7	16
210	106-41-2	4-Bromophenol	9.2	4.2	8.7
211	106-42-3	p-Xylene	9.6	6.9	11
212	106-43-4	p-Chlorotoluene	6.1	2.0	6.1
213	106-44-5	p-Cresol	52	7.0	14
214	106-46-7	p-Dichlorobenzene	5.4	2.5	2.2
215	106-47-8	p-Chloroaniline	3.8	0.31	5.8
216	106-48-9	p-Chlorophenol	10	2.5	8.9
217	106-49-0	p-Toluidine	24	1.3	120
218	106-50-3	p-Phenylenediamine	0.18	0.33	0.066
219	106-87-6	7-Oxa-3-oxiranylbicyclo[4.1.0]heptane	-	58 ^a	15 ^b
220	106-91-2	Glycidyl methacrylate	32	25	2.8
221	107-06-2	1,2-Dichloroethane	230	99	>130
222	107-13-1	2-Propenenitrile	10	2.5	5.1
223	107-18-6	Allyl alcohol	>10	2.1	0.59
224	107-21-1	Ethylene glycol	>1000	>1100	>100
225	107-41-5	Hexylene glycol	>1000	>1000	>100
226	108-05-4	Vinyl acetate	8.9	9.2	2.4
227	108-20-3	Isopropyl ether	>97	-	-
228	108-38-3	m-Xylene	8.9	2.4	19
229	108-42-9	m-Chloroaniline	19	0.49	8.8
230	108-45-2	m-Phenylenediamine	30	2.0	-
231	108-65-6	2-Methoxy-1-methylethyl acetate	>1000	370	>100
232	108-69-0	3,5-Dimethylaniline	29	2.2	34
233	108-70-3	1,3,5-Trichlorobenzene	>4.8	2.9	3.2
234	108-80-5	Isocyanuric acid	950	1000	>100
235	108-86-1	Bromobenzene	12	-	4.3
236	108-87-2	Methylcyclohexane	0.34	0.33	2.1
237	108-88-3	Toluene	29	4.1	25
238	108-90-7	Chlorobenzene	-	-	6.6 ^b
239	108-91-8	Cyclohexylamine	34	36	33
240	108-95-2	Phenol	160	15	25
241	108-98-5	Benzenethiol	0.16	0.0044	0.009
242	108-99-6	3-Methylpyridine	>32	34	-
243	109-59-1	2-Isopropoxyethanol	>1000	>1000	>100
244	109-64-8	1,3-Dibromopropane	46	8.8	7.8
245	109-86-4	2-Methoxyethanol	>100	>85	>89
246	109-89-7	Diethylamine	54	58	27
247	110-00-9	Furan	>58	110	-
248	110-02-1	Thiophene	110	21	31
249	110-19-0	Isobutyl acetate	370	25	17

250	110-26-9	N,N'-Methylenediacrylamide	-	-	240 ^b
251	110-30-5	Octadecanoylaminoethyl)octadecanamide	>0.053	>0.0022	>0.027
252	110-44-1	Sorbic acid	85	70	75
253	110-62-3	Valeraldehyde	>9.3	32	13
254	110-63-4	1,4-Butanediol	>1000	>1000	>100
255	110-66-7	Pentane-1-thiol	0.14	0.027	1.3
256	110-75-8	2-Chloroethyl vinyl ether	-	-	>99 ^b
257	110-80-5	2-Ethoxyethanol	>100	>90	>95
258	110-81-6	Diethyl disulfide	4.4	0.39	12
259	110-83-8	Cyclohexene	>3.6	2.1	5.8
260	110-85-0	Piperazine	130	110	>100
261	110-86-1	Pyridine	0.1	180	-
262	110-91-8	Morpholine	58	45	-
263	111-03-5	2,3-Dihydroxypropyl oleate	>130	49	>100
264	111-14-8	Heptanoic acid	60	72	75
265	111-15-9	2-Ethoxyethyl acetate	>1000	200	42
266	111-17-1	3,3'-Thiodipropionic acid	50	73	>99
267	111-18-2	N,N,N',N'-Tetramethylhexamethylenediamine	71	78	-
268	111-30-8	Glutaraldehyde	1.9	8.7	8.8
269	111-44-4	Bis(2-chloroethyl) ether	340	410	>100
270	111-65-9	Octane	>1.1	0.18	0.42
271	111-70-6	1-Heptanol	34	56	18
272	111-76-2	Ethylene glycol monobutyl ether	>1000	>1000	>100
273	111-78-4	1,5-Cyclooctadiene	8.2	0.87	13
274	111-82-0	Methyl dodecanoate	0.32	0.23	>0.52
275	111-85-3	1-Chlorooctane	>0.27	0.21	0.62
276	111-88-6	1-Mercaptooctane <n-Octylmercaptan>	0.014	0.024	0.33
277	112-12-9	2-Undecanone	1.9	1.3	-
278	112-30-1	1-Decanol	0.56	1.4	2.8
279	112-41-4	Dodec-1-ene	>0.097	0.38	2.6
280	112-57-2	Tetraethylenepentamine	0.12	13	>70
281	112-70-9	Tridecan-1-ol	0.012	0.61	1.7
282	112-80-1	Oleic acid	>2.6	>2.8	>2.5
283	112-85-6	Docosanoic acid	>4.1	>5.0	>5.0
284	113-48-4	N-(2-Ethylhexyl)-8,9,10-trinorborn-5-ene-2,3-dicarboximide	-	3.6 ^a	2.0 ^b
285	115-32-2	Kelthane	>19	0.096	0.28
286	115-70-8	2-Amino-2-ethylpropanediol	51	>97	>97
287	117-08-8	Tetrachlorophthalic anhydride	84	-	-
288	117-80-6	2,3-Dichloro-1,4-naphthoquinone	0.072	0.017	0.031
289	117-81-7	Bis(2-ethylhexyl) phthalate	>100	>100	-
290	117-84-0	Dioctyl phthalate	-	>0.00067 ^a	-
291	118-69-4	2,6-Dichlorotoluene	2.7	0.38	2.3
292	118-79-6	2,4,6-Tribromophenol	1.9	2.2	1.5
293	119-06-2	Ditridecyl phthalate	>50	>50	>50
294	119-12-0	pyridazin-6-yl) phosphorothionate	>8.5	0.00051	>10
295	119-34-6	4-Amino-2-nitrophenol	5.0	2.2	-
296	119-47-1	6,6'-Di-tert-butyl-2,2'-methylenedi-p-cresol	>4.5	>4.8	>5.0
297	119-61-9	Benzophenone	3.5	>10	>10
298	119-64-2	Tetrahydronaphthalene	-	-	6.0 ^b
299	119-93-7	o-Tolidine	6.3	4.5	13

300	120-12-7	Anthracene	>0.031	>0.031	>0.03
301	120-61-6	Dimethyl terephthalate	>5.3	>6.5	>5.4
302	120-82-1	1,2,4-Trichlorobenzene	5.7	1.4	2.4
303	120-83-2	2,4-Dichlorophenol	4.8	2.2	3.4
304	120-95-6	2,4-Di-tert-pentylphenol	1.7	0.12	0.29
305	121-44-8	Triethylamine	8.0	34	24
306	122-34-9	6-Chloro-N,N'-diethyl-1,3,5-triazine-2,4-diamine <Simazine>	-	-	>4.6 ^b
307	122-39-4	Diphenylamine	0.43	1.5	6.6
308	122-40-7	Amylcinnamic aldehyde	>1.5	0.28	0.91
309	122-57-6	Benzalacetone	0.55	15	5.7
310	122-66-7	Hydrazobenzene	1.1	1.1	0.043
311	123-11-5	p-Methoxybenzaldehyde	61	45	40
312	123-15-9	2-Methylvaleraldehyde	6.0	15	-
313	123-30-8	4-Aminophenol	0.1	0.32	0.93
314	123-31-9	Hydroquinone	0.053	0.061	-
315	123-35-3	7-Methyl-3-methyleneocta-1,6-diene	>1.6	0.45	0.92
316	123-39-7	N-Methylformamide	>1000	>1000	>100
317	123-42-2	Diacetone alcohol	>1000	>1000	>100
318	123-91-1	1,4-Dioxane	>1000	>1000	>100
319	124-04-9	Adipic acid	59	46	-
320	124-07-2	Octanoic acid	39	63	51
321	124-09-4	1,6-Hexanediamine	19	27	71
322	124-28-7	Dimantine	0.0018	0.016	0.079
323	124-48-1	Dibromochloromethane	9.6	27	79
324	126-33-0	Sulfolane	>1000	850	>100
325	126-98-7	Methacrylonitrile	25	250	-
326	127-18-4	Tetrachloroethylene	27	1.3	14
327	127-90-2	2,3,3,3,2',3',3',3'-Octachlorodipropyl ether	1.2	0.078	0.59
328	128-37-0	2,6-Di-tert-butyl-4-methylphenol	>7.0	0.84	1.1
329	129-00-0	Pyrene	>2.7	1.6	1.0
330	131-17-9	Diallyl phthalate	15	16	0.44
331	131-57-7	2-Hydroxy-4-methoxybenzophenone	0.67	1.9	3.8
332	132-65-0	Dibenzothiophene	1.4	0.44	1.4
333	134-62-3	N,N-Diethyl-m-toluamide	>100	74	-
334	134-96-3	4-Hydroxy-3,5-dimethoxybenzaldehyde	-	42 ^a	-
335	135-19-3	2-Naphthol	2.1	5.3	4.0
336	135-57-9	Bis(2-benzoylaminophenyl)disulfide	>0.025	>0.032	>0.042
337	138-52-3	.beta.-D-Glucopyranoside, 2-(hydroxymethyl)phenyl	-	>5000 ^a	>5100 ^b
338	138-86-3	p-Mentha-1,8-diene	>1.6	0.7	1.1
339	140-66-9	4-t-Octylphenol	-	-	0.36
340	139-13-9	Nitrilotriacetic acid	>30	110	-
341	140-88-5	Ethyl acrylate	2.3	4.4	1.2
342	141-32-2	n-Butyl acrylate	1.7	5.2	2.4
343	141-43-5	Monoethanolamine	2.5	97	-
344	142-96-1	Butane, 1,1'-oxybis-	22	17	-
345	143-07-7	Lauric acid	>6.2	3.6	5.0
346	143-08-8	1-Nonanol	2.2	3.9	3.2
347	143-10-2	1-Decanethiol	0.0078	0.01	>0.053
348	143-22-6	Triethylene glycol monobutyl ether	>920	-	-
349	144-62-7	Oxalic acid	22	15	27

350	145-39-1	1-tert-Butyl-3,4,5-trimethyl-2,6-dinitrobenzene	-	>0.042 ^a	>0.045 ^b
351	148-24-3	8-Hydroxyquinoline	0.52	1.7	2.5
352	149-30-4	2-Mercaptobenzothiazole	0.5	0.71	>2.8
353	156-59-2	cis-1,2-Dichloroethene cis-1,2-Dichloroethylene	>74	40	67
354	193-39-5	Indeno[1,2,3-cd]pyrene	0.0002	0.0013	>0.0037
355	205-82-3	Benzo[<i>jj</i>]fluoranthene	>0.00026	0.0023	>0.0042
356	286-62-4	Cyclooctene oxide	-	24 ^a	200 ^b
357	298-06-6	O,O-Diethyldithio phosphate	>100	4.5	66
358	298-12-4	Glyoxylic acid	33	51	41
359	302-17-0	2,2,2-Trichloroethane-1,1-diol	>95	>98	>96
360	334-48-5	Decanoic acid	12	>20	>16
361	348-61-8	4-Bromo-1,2-difluorobenzene	14	6.3	7.8
362	350-30-1	2-Chloro-1-fluoro-4-nitrobenzene	0.6	8.2	2.0
363	352-87-4	2,2,2-Trifluoroethyl methacrylate	-	22 ^a	8.3 ^b
364	374-25-4	1-Butene, 4-bromo-3-chloro-3,4,4-trifluoro-	-	2.5 ^a	-
365	394-50-3	3-Fluoro-2-hydroxybenzaldehyde	-	9.9 ^a	-
366	402-31-3	Metaxylene hexafluoride	7.8	3.9	7.3
367	406-86-0	4,4,4-Trifluorocrotonitrile	0.36	0.37	0.2
368	461-58-5	Cyanoguanidine	>1000	>1000	>100
369	462-08-8	3-Aminopyridine	0.25	7.1	8.6
370	464-72-2	1,1,2,2-Tetraphenylethane-1,2-diol	-	0.017 ^a	>0.043 ^b
371	470-82-6	2-Oxabicyclo[2.2.2]octane, 1,3,3-trimethyl-	250	200	-
372	479-27-6	1,8-Naphthylenediamine	0.48	0.17	5.6
373	483-63-6	N-Ethyl-N-crotonoyl-2-toluidine	-	-	75 ^b
374	487-68-3	2,4,6-Trimethylbenzaldehyde	7.9	4.5	12
375	497-18-7	Carbonohydrazide	9.5	52 ^a	-
376	504-24-5	4-Aminopyridine	30	15	3.4
377	504-29-0	2-Aminopyridine	12	35	11
378	505-32-8	3,7,11,15-Tetramethylhexadec-1-en-3-ol	>20	11	>20
379	515-84-4	Ethyl trichloroacetate	70	160	44
380	534-52-1	4,6-Dinitro-o-cresol	5.6	1.7	1.1
381	535-13-7	Ethyl 2-chloropropionate	-	30 ^a	-
382	541-73-1	m-Dichlorobenzene	>6.3	2.5	5.7
383	542-75-6	1,3-Dichloropropene	2.1	1.2	1.5
384	544-01-4	Diisopentyl ether	>4.4	2.3	6.8
385	544-63-8	Myristic acid	>2.1	>1.7	>1.9
386	545-06-2	Trichloroacetonitrile	-	0.044 ^a	0.072 ^b
387	554-00-7	2,4-Dichloroaniline	>9.9	4.2	8.1
388	555-03-3	m-Nitroanisole	18	19	59
389	556-61-6	Methyl isothiocyanate	0.19	0.12	0.12
390	556-82-1	3-Methylbut-2-en-1-ol	>870	170	47
391	573-98-8	1,2-Dimethylnaphthalene	4.1	1.1	2.3
392	575-41-7	1,3-Dimethylnaphthalene	0.62	0.98	1.8
393	576-26-1	2,6-Xylenol	48	11	15
394	581-42-0	2,6-Dimethylnaphthalene	>4.4	2.5	>9.2
395	582-16-1	2,7-Dimethylnaphthalene	1.0	1.5	1.8
396	591-27-5	3-Aminophenol	160	0.45	120
397	593-08-8	2-Tridecanone	0.12	0.0081	-
398	599-64-4	4-(a,a-Dimethylbenzyl)phenol	1.4	1.7	1.2
399	606-20-2	2,6-Dinitrotoluene	15	20	34
400	611-19-8	2-Chlorobenzyl chloride	1.2	0.38	0.27

401	615-58-7	2,4-Dibromophenol	1.1	2.1	3.6
402	619-24-9	3-Nitrobenzonitrile	-	92 ^a	42 ^b
403	620-92-8	4,4'-Dihydroxydiphenylmethane	16	12	13
404	620-93-9	Di-p-tolylamine	0.14	0.4	0.43
405	623-15-4	4-(2-Furyl)but-3-en-2-one	-	13 ^a	21 ^b
406	624-92-0	Dimethyl disulphide	29	5.7	1.1
407	629-40-3	Octanedinitrile	120	370	550
408	634-93-5	2,4,6-Trichloroaniline	3.7	4.3	5.3
409	638-16-4	1,3,5-Triazine-2,4,6-trithiol	>95	38	-
410	674-82-8	But-3-en-3-olide	6.9	2.6	8.8
411	683-10-3	1-Dodecanaminium, N-(carboxymethyl)-N,N-dimethyl-, inner salt	3.8	2.0	0.88
412	688-84-6	2-Ethylhexyl methacrylate	5.3	4.6	2.8
413	691-37-2	4-methylpent-1-ene	>0.0074	>0.082	>0.076
414	693-54-9	2-Decanone	4.9	3.5	-
415	693-98-1	2-Methylimidazole	-	200 ^a	-
416	716-79-0	1H-Benzimidazole, 2-phenyl-	-	4.2 ^a	8.6 ^b
417	732-26-3	2,4,6-Tri-tert-butylphenol	>0.32	0.11	>10
418	760-23-6	3,4-Dichlorobut-1-ene	58	10	27
419	763-69-9	Ethyl 3-ethoxypropionate	>86	>92	>93
420	764-13-6	2,5-Dimethylhexa-2,4-diene	>4.7	4.2	2.6
421	764-42-1	2-Butenedinitrile, (E)-	0.38	0.33	0.36
422	782-74-1	1,2-Bis(2-chlorophenyl)hydrazine	>2.5	0.23	0.1
423	793-24-8	N-1,3-Dimethylbutyl-N'-phenyl-p-phenylenediamine	-	0.23 ^a	0.029 ^b
424	818-61-1	2-Hydroxyethyl acrylate	6.0	5.2	6.5
425	827-43-0	4-Methyl-2-phenyl-1H-imidazole	-	44 ^a	45 ^b
426	827-52-1	Cyclohexylbenzene	0.69	0.37	1.2
427	839-90-7	Tris(2-hydroxyethyl)-1,3,5-triazinetriene	>1000	>1000	>100
428	840-65-3	Dimethyl naphthalene-2,6-dicarboxylate	>0.025	>0.10	>0.10
429	843-55-0	1,1-Bis(4-hydroxyphenyl)-cyclohexane	>3.6	1.8	1.8
430	868-63-3	N,N'-(1,2-Dihydroxy-1,2-ethanediyl) bisacrylamide	-	-	110 ^b
431	868-77-9	2-Hydroxyethyl methacrylate	710	380	>100
432	873-32-5	o-Chlorobenzonitrile	19	18	37
433	882-33-7	Phenyl disulfide	>0.019	0.0085	0.058
434	892-21-7	3-Nitrofluoranthene	>0.23	>0.33	>0.29
435	901-44-0	2,2-Bis[4-(2-hydroxyethoxy)phenyl]propane	17	>34	21
436	920-37-6	2-Propenenitrile, 2-chloro-	0.069	0.078	0.084
437	924-41-4	1,5-Hexadien-3-ol	-	26 ^a	-
438	947-04-6	Dodecane-12-lactam	>100	65	55
439	948-65-2	2-Phenylindole	0.2	0.3	0.27
440	1014-70-6	2,4-Bis(ethylamino)-6-methylthio-1,3,5-triazine	0.028	>10	>10
441	1025-15-6	Triallyl isocyanurate	-	-	>95 ^b
442	1116-76-3	Tri-n-octylamine	0.0022	0.026	>0.045
443	1118-61-2	2-Butenenitrile, 3-amino-	3.3	34	17
444	1120-21-4	n-Undecane	>0.0059	0.011	>0.013
445	1151-97-9	2-[(2,4-Dinitrophenyl)methyl]pyridine	-	23 ^a	23 ^b
446	1163-19-5	Decabromodiphenyl Oxide	>0.0052	>0.0048	>0.0046
447	1191-39-5	N-Dodecylmethacrylamide	-	-	>0.11 ^b
448	1321-74-0	Divinylbenzene	1.8	1.9	4.2
449	1335-46-2	Methylionone	-	3.1 ^a	3.0 ^b
450	1338-41-6	Sorbitan, mono-octadecanoate	>56	>13	>6.3

451	1477-55-0	m-Phenylenebis(methylamine)	28	15	88
452	1484-13-5	9-Vinylcarbazole	0.021	0.0006	-
453	1502-22-3	2-(1'-Cyclohexenyl)cyclohexanone	19	20	29
454	1540-36-9	2,4-Pentanedione, 3-butyl-	-	-	210 ^b
455	1620-98-0	3,5-Di-tert-butyl-4-hydroxybenzaldehyde	-	>0.18 ^a	-
456	1634-04-4	Methyl t-butyl ether	>110	>120	>120
457	1643-20-5	Dodecyldimethylamine oxide	0.11	2.2	30
458	1667-10-3	4,4'-Bis(chloromethyl)biphenyl	>0.30	>0.0022	>0.0023
459	1678-91-7	Ethylcyclohexane	0.63	0.67	0.75
460	1806-26-4	p-Octylphenol	0.14	0.42	0.088
461	1843-05-6	2-Hydroxy-4-n-octyloxybenzophenone	>0.0021	>0.0038	>0.0036
462	1855-63-6	1-Cyclohexene-1-carbonitrile	41	48	41
463	1879-09-0	2-(1,1-Dimethylethyl)-4,6-dimethylphenol	7.1	2.9	2.5
464	1953-99-7	3,4,5,6-Tetrachlorobenzene-1,2-dicarbonitrile	-	0.3 ^a	0.12 ^b
465	1989-32-8	9-(Dicyanomethylene)fluorene	-	-	>0.24 ^b
466	2100-42-7	2-Chlorohydroquinonedimethylether	10	17	28
467	2219-82-1	6-Tert-butyl-o-cresol	6.3	5.3	4.3
468	2232-08-8	1-(p-Toluenesulphonyl)imidazole	-	35 ^a	-
469	2243-62-1	1,5-Naphthalenediamine	2.1	3.8	17
470	2403-88-5	2,2,6,6-Tetramethylpiperidin-4-ol	120	100	>100
471	2409-55-4	2-tert-Butyl-p-cresol	1.8	2.7	1.9
472	2425-79-8	1,4-Bis(2,3-epoxypropoxy)butane	>93	22	13
473	2437-25-4	Dodecanenitrile	0.15	0.059	0.84
474	2439-01-2	6-Methyl-1,3-dithiolo[4,5-b]quinoxalin-2-one	0.097	0.016	-
475	2439-35-2	2-(Dimethylamino)ethyl acrylate	>1.0	9.9	8.5
476	2465-27-2	4,4'-(Iminomethylene)bis(N,N-dimethylaniline) monohydrochloride	0.34	4.6	6.0
477	2479-46-1	4,4'-(m-Phenylenedioxy)dianiline	>2.2	2.9	1.9
478	2486-13-7	2,4-Dinitrostilbene	-	>0.065 ^a	>0.059 ^b
479	2840-28-0	3-Amino-4-chlorobenzoic acid	11	6.9	>97
480	2867-47-2	2-(Dimethylamino)ethyl methacrylate	9.0	33	19
481	3006-82-4	tert-Butyl 2-ethylperoxyhexanoate	0.3	3.9	4.6
482	3030-47-5	N-Methyl-N,N-bis(2-dimethylaminoethyl)amine	52	51	-
483	3048-65-5	3a,4,7,7a-Tetrahydro-1H-indene	7.0	0.73	4.4
484	3268-49-3	3-(Methylthio)propionaldehyde	0.99	7.2	7.0
485	3278-89-5	2-(Allyloxy)-1,3,5-tribromobenzene	-	>0.019 ^a	>0.025 ^b
486	3295-94-1	Allyl n-hexyl ether	-	2.4 ^a	4.9 ^b
487	3380-34-5	Triclosan	0.0034	0.27	0.67
488	3452-97-9	3,5,5-Trimethyl-1-hexanol	>33	6.8	28
489	3648-21-3	Diheptyl phthalate	>1000	0.37	-
490	3695-93-0	Alpha-(p-chlorophenyl)cinnamionitrile	-	-	>0.049 ^b
491	3766-81-2	2-sec-Butylphenyl N-methylcarbamate	33	0.014	9.8
492	3984-22-3	2-Vinyl-1,3-dioxolane	-	-	65 ^b
493	4067-16-7	Pentaethylenehexamine	0.42	8	210
494	4130-42-1	2,6-Di-tert-Butyl-4-ethylphenol	>0.52	>0.47	0.59
495	4170-30-3	Crotonaldehyde	0.94	1.0	0.072
496	4286-23-1	4-(1-Methylethenyl)phenol	5.4	4.1	9.2
497	4418-61-5	5-Aminotetrazole	>99	17	-
498	4457-71-0	3-Methyl-1,5-pentanediol	>1000	>1000	>100
499	4798-44-1	1-Hexen-3-ol	-	210 ^a	-
500	4979-32-2	N,N-Dicyclohexylbenzothiazole-2-sulphenamide	>0.012	>0.031	>0.033

501	5329-12-4	2,4,6-Trichlorophenylhydrazine	0.084	1.3	1.0
502	5405-58-3	Hexane, 1,1 -[ethylidenebis(oxy)]bis-	>0.43	0.28	>0.59
503	5432-07-5	Benzene, 1-methoxy-4-(2-cyano-2-phenylethenyl)-	-	-	>0.24 ^b
504	5510-99-6	2,6-Di-sec-butylphenol	1.1	0.96	0.15
505	5522-43-0	1-Nitropyrene	>0.0053	>0.33	>0.33
506	5707-44-8	1,1'-Biphenyl, 4-ethyl- <4-Ethyl-1,1'-biphenyl>	0.15	0.27	0.6
507	6117-91-5	2-Buten-1-ol	-	5.6 ^a	4.0 ^b
508	6165-51-1	2-(1-Phenylethyl)-p-xylene	>1.5	0.25	0.31
509	6362-80-7	2,4-Diphenyl-4-methylpentene-1	>0.059	0.057	>0.092
510	6807-17-6	4,4-Isobutylethylidendiphenol	>17	13	2.7
511	6842-15-5	1-Propene, tetramer	>0.0032	0.015	>0.014
512	6864-37-5	2,2'-Dimethyl-4,4'-methylenebis(cyclohexylamine)	6.1	4.6	22
513	7212-44-4	1,6,10-Dodecatrien-3-ol, 3,7,11-trimethyl-	-	0.96 ^a	-
514	7299-99-2	Hexanoic acid, 2-ethyl-, 2,2-bis[[(2-ethyl-1-oxohexyl)oxy]methyl]-1,3-propanediyl ester	>0.020	>0.012	>0.048
515	7580-85-0	2-t-Butoxyethanol	>870	>1000	>100
516	9002-93-1	Polyethylene glycol mono[4-(1,1,3,3-tetramethylbutyl)phenyl]ether	>220	14	24
517	9014-90-8	α-Sulfo-ω-(nonylphenoxy)-poly(oxy-1,2-ethanediyl), sodium salt	380	21	25
518	10500-57-9	5,6,7,8-Tetrahydroquinoline	64	11	37
519	11070-44-3	Tetrahydromethylphthalic anhydride	81	130	-
520	13048-33-4	Hexamethylene diacrylate	1.6	2.7	0.38
521	13481-25-9	2,3-Pyrazinedicarbonitrile	-	2.1 ^a	2.0 ^b
522	13826-35-2	Benzyl alcohol, 3-phenoxy-	-	1.5 ^a	3.8 ^b
523	14802-03-0	2-Ethylhexyl hydrogen (2-ethylhexyl) phosphonate	92	43	98
524	14938-35-3	4-Pentylphenol	2.2	0.9	1.4
525	15045-43-9	2,2,5,5-Tetramethyltetrahydrofuran	590	200	-
526	16219-75-3	5-Ethylidene-8,9,10-trinorborn-2-ene	4.9	3.3	7.0
527	16245-79-7	4-Octylbenzenamine	-	0.03 ^a	-
528	16669-59-3	N-(Isobutoxymethyl)acrylamide	-	-	60 ^b
529	16691-43-3	3-Amino-5-mercapto-1H-1,2,4-triazole	>100	0.53	-
530	17796-82-6	N-(Cyclohexylthio)phthalimide	>0.10	>2.0	>2.0
531	18375-66-1	N-Octadecyl-D-gluconamide	>0.01	>0.01	>0.01
532	18854-01-8	Isoxathion	0.87	0.00019	-
533	19398-61-9	2,5-Dichlorotoluene	1.7	1.1	4.0
534	19715-19-6	3,5-Di-tert-butylsalicylic acid	6.8	3.2	2.7
535	20103-09-7	2,5-Dichloro-1,4-benzenediamine	-	0.85 ^a	22 ^b
536	21087-64-9	Metribuzin	0.039	88	-
537	22509-74-6	N-Carboethoxyphthalimide	-	>8.7 ^a	1.4 ^b
538	22720-75-8	1-Benzo[b]thien-2-ylethan-1-one	5.4	11	10
539	23184-66-9	N-(Butoxymethyl)-2-Chloro-2',6'-diethylacetanilide	0.0033	1.9	0.28
540	23950-58-5	Propyzamide	3.4	>10	>9.8
541	25013-16-5	Butylated hydroxyanisole	5.2	2.3	5.8
542	25103-58-6	tert-Dodecanethiol	>4.1	0.075	0.38
543	25321-09-9	Diisopropylbenzene	3.4	0.39	0.71
544	25339-17-7	Isodecyl alcohol	6.8	3.5	5.9
545	25377-73-5	Dodecenylsuccinic anhydride	>1.2	13	3.8
546	25675-28-9	1-(3-Methylphenyl)ethanol	-	-	170 ^b
547	25973-55-1	Phenol, 2-(2H-benzotriazol-2-yl)-4,6-bis(1,1-dimethylpropyl)-	>0.016	>0.083	>0.078

548	26544-23-0	Diphenyl isodecyl phosphite	>0.24	>0.22	>0.24
549	27955-94-8	Phenol, 4,4',4''-ethylidynetris-	3.9	>20	>17
550	28249-77-6	S-4-Chlorobenzyl diethylthiocarbamate	0.092	1.3	1.3
551	29082-74-4	Octachlorostyrene	>2.6	0.0058	>3.5
552	29253-36-9	Isopropyl naphthalene	0.25	0.15	0.74
553	30171-80-3	Dibromocresyl glycidyl ether	0.61	1.3	1.3
554	31127-54-5	2,3,4,4'-Tetrahydroxybenzophenon	0.54	39	36
555	32388-55-9	Ethanone, 1-[(3R,3aR,7R,8aS)-2,3,4,7,8,8a-hexahydro-3,6,8,8-tetramethyl-1H-3a,7-methanoazulen-5-yl]-	>0.16	>0.48	>0.42
556	32536-52-0	Octabromodiphenyl ether	>0.012	>0.011	>0.012
557	37721-71-4	2,4,6-Tribromophenyl methacrylate	-	>0.13 ^a	>0.12 ^b
558	38640-62-9	Diisopropyl naphthalene	>0.071	0.035	>0.093
559	40220-08-4	Tris(2-hydroxyethyl)isocyanuric acid	26	87	6.8
560	41122-70-7	4'-Hexyl[1,1'-biphenyl]-4-carbonitrile	-	0.0076 ^a	>0.014 ^b
561	41451-28-9	Diisoheptyl phthalate	>1000	0.39	>100
562	42152-47-6	7-Methyl-1,6-octadiene	>0.022	>0.51	>0.52
563	45206-91-5	Hexadecan-7-one	>0.016	>0.0040	>0.0034
564	50512-35-1	Diisopropyl 1,3-dithiolan-2-ylidenemalonate	>10	>10	9.3
565	51218-49-6	2-Chloro-2',6'-diethyl-N-(2-propoxyethyl)acetanilide	0.0032	7.0	2.4
566	51963-82-7	Benzenamine, 2,5-diethoxy-4-(4-morpholinyl)-	7.4	18	22
567	52829-07-9	Bis(2,2,6,6-tetramethyl-4-piperidyl)	1.1	8.6	5.3
568	56539-66-3	3-Methoxy-3-methyl-1-butanol	>1000	>1000	>100
569	57500-00-2	Furfuryl methyl disulfide	-	0.31 ^a	-
570	61788-44-1	Mono (or di or tri)-(.alpha.-methylbenzyl) phenol	>10	4.6	5.6
571	68972-96-3	cis-1,4-Dibenzyloxy-2-butene	-	1.4 ^a	4.6 ^b
572	76334-36-6	3-Bromo-3-buten-1-ol	-	69 ^a	-
573	70974-33-3	Benzenesulfonic acid, 4-hydroxy-,	3.2	-	>97
574	76334-36-6	3-Bromo-3-buten-1-ol	-	-	43
575	85068-29-7	3,5-Bis(trifluoromethyl)benzylamine	3.6	5.5	11
576	85785-20-2	ethylthiocarbamate	>0.081	0.15	1.3
577	88613-26-7	2-(p-Nitrophenoxy)ethyl methacrylate	-	>6.4 ^a	>7.5 ^b

^achemical not included in algae(*P. subcapitata*) data; ^bchemical not included in algae(*P. subcapitata*) data

Table S2: External test data set. Reprinted from Sci. Total Environ., Vol. 408, Xu J. Zhang, Hong W. Qin, Li M. Su, Wei C. Qin, Ming Y. Zou, Lian X. Sheng, Yuan H. Zhao, Michael H. Abraham, Multi-species QSAR modeling for predicting aquatic toxicity of diverse organic chemicals for regulatory toxicology, 4549-4555, Copyright 2010, with permission from Elsevier.

S.No.	SMILES	CAS	Name	15min- log1/EC ₅₀ (V.fischeri,mol/l)	48h- log1/EC ₅₀ (Algae,mol/l)
1	CC(C)=O	000067-64-1	Acetone	0.90 ^a	-
2	CCOCC	000060-29-7	Diethyl ether	1.68 ^a	-
3	C1CCOC1	000109-99-9	Tetrahydrofuran	1.90 ^a	-
4	CCCCCC	000110-54-3	Hexane	3.27 ^a	-
5	C1CCCCC1	000110-82-7	Cyclohexane	3.16 ^a	-
6	CCCCCCCCO	000111-87-5	1-Octanol	4.90 ^a	-
7	O=C1CCCCC1	000108-94-1	Cyclohexanone	2.95 ^a	-
8	ClCCl	000075-09-2	Dichloromethane	1.96 ^a	-
9	ClC(Cl)Cl	000067-66-3	Chloroform	2.55 ^a	-
10	ClCCCl	000107-06-2	1,2-Dichloroethane	2.43	-
11	ClC(Cl)C(Cl)Cl	000079-34-5	1,1,2,2-Tetrachloroethane	3.70 ^a	-
12	ClC(Cl)(Cl)C(Cl)(Cl)Cl	000067-72-1	Hexachloroethane	5.52 ^a	-
13	ClC(Cl)=C(Cl)Cl	000127-18-4	Tetrachloroethylene	3.94	-
14	c1ccccc1	000071-43-2	Benzene	3.34 ^a	-
15	Cc1ccccc1	000108-88-3	Toluene	3.08	-
16	Cc1c(C)cccc1	000095-47-6	2-Xylene	4.08 ^a	-
17	Cc1cc(C)ccc1	000108-38-3	3-Xylene	3.65 ^a	-
18	Cc1ccc(C)cc1	000106-42-3	4-Xylene	3.68 ^a	-
19	Clc1ccccc1	000108-90-7	Chlorobenzene	3.86 ^a	-
20	BrC1ccccc1	000108-86-1	Bromobenzene	3.78	-
21	Clc1ccc(C)cc1	000106-43-4	4-Chlorotoluene	3.88 ^a	-
22	Clc1ccccc1Cl	000095-50-1	1,2-Dichlorobenzene	4.38 ^a	-
23	Clc1cccc(Cl)c1	000541-73-1	1,3-Dichlorobenzene	4.24 ^a	-
24	Clc1ccc(Cl)cc1	000106-46-7	1,4-Dichlorobenzene	4.39 ^a	-
25	BrC1cc(Br)ccc1	000108-36-1	1,3-Dibromobenzene	4.99 ^a	-
26	BrC1ccc(Br)cc1	000106-37-6	1,4-Dibromobenzene	4.54 ^a	-
27	Clc1ccc(Br)cc1	000106-39-8	4-Bromochlorobenzene	4.50 ^a	-
28	Clc1c(C)cc(Cl)cc1	019398-61-9	2,5-Dichlorotoluene	4.38	-
29	Clc1cccc(Cl)c1Cl	000087-61-6	1,2,3-Trichlorobenzene	4.53	-
30	Clc1ccc(Cl)c(Cl)c1	000120-82-1	1,2,4-Trichlorobenzene	4.5	-

31	<chem>Clc1c(C)cc(Cl)c(Cl)c1</chem>	006639-30-1	2,4,5-Trichlorotoluene	4.86 ^a	-
32	<chem>Clc1cc(Cl)c(Cl)cc1Cl</chem>	000095-94-3	1,2,4,5-Tetrachlorobenzene	5.51 ^a	-
33	<chem>Clc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl</chem>	000118-74-1	Hexachlorobenzene	6.32 ^a	-
34	<chem>Nc1ccccc1</chem>	000062-53-3	Aniline	3.28	2.56
35	<chem>Cc1ccccc1N</chem>	000095-53-4	2-Methylaniline	-	2.34 ^b
36	<chem>Nc1ccc(C)cc1</chem>	000106-49-0	4-Methylaniline	-	3.19 ^b
37	<chem>Clc1ccccc1N</chem>	000095-51-2	2-Chloroaniline	-	2.89 ^b
38	<chem>Nc1cc(Cl)ccc1</chem>	000108-42-9	3-Chloroaniline	-	2.79 ^b
39	<chem>Nc1ccc(Cl)cc1</chem>	000106-47-8	4-Chloroaniline	3.57 ^a	-
40	<chem>Nc1cc(Br)ccc1</chem>	000591-19-5	3-Bromoaniline	-	2.80 ^b
41	<chem>c1cc(N)ccc1Br</chem>	000106-40-1	4-Bromoaniline	3.92 ^a	-
42	<chem>Nc1ccc(F)c(Cl)c1</chem>	000367-21-5	3-Chloro-4-fluoroaniline	3.28 ^a	-
43	<chem>Nc1cccc(Cl)c1Cl</chem>	000608-27-5	2,3-Dichloroaniline	-	3.98 ^b
44	<chem>Nc1ccc(Cl)cc1Cl</chem>	000554-00-7	2,4-Dichloroaniline	4.09	3.74
45	<chem>Nc1cc(Cl)ccc1Cl</chem>	000095-82-9	2,5-Dichloroaniline	-	3.82
46	<chem>Nc1c(Cl)cccc1Cl</chem>	000608-31-1	2,6-Dichloroaniline	4.16 ^a	-
47	<chem>Nc1ccc(Cl)c(Cl)c1</chem>	000095-76-1	3,4-Dichloroaniline	4.2	-
48	<chem>Nc1c(Cl)cc(Cl)cc1Cl</chem>	000634-93-5	2,4,6-Trichloroaniline	4.51	-
49	<chem>Nc1c(Br)cc(Br)cc1Br</chem>	000147-82-0	2,4,6-Tribromoaniline	-	4.37 ^b
50	<chem>N(c1ccccc1)c2ccccc2</chem>	000122-39-4	Diphenylamine	4.88	-
51	<chem>Oc1ccccc1</chem>	000108-95-2	Phenol	3.64	2.46
52	<chem>Cc1c(O)cccc1</chem>	000095-48-7	2-Methylphenol	3.75 ^a	-
53	<chem>Oc1ccccc1Cl</chem>	000095-57-8	2-Chlorophenol	4.14 ^a	-
54	<chem>Clc1ccc(O)cc1</chem>	000106-48-9	4-Chlorophenol	4.48 ^a	-
55	<chem>Oc1ccc(Cl)cc1Cl</chem>	000120-83-2	2,4-Dichlorophenol	4.45	3.62
56	<chem>Oc1c(Cl)cc(Cl)cc1Cl</chem>	000088-06-2	2,4,6-Trichlorophenol	-	3.81 ^b
57	<chem>Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl</chem>	000087-86-5	Pentachlorophenol	5.69	4.63
58	<chem>Oc1cccc(O)c1</chem>	000108-46-3	Resorcinol	3.00 ^a	-
59	<chem>c1cc([N+](=O)[O-])ccc1</chem>	000098-95-3	Nitrobenzene	3.82 ^a	3.26 ^b
60	<chem>[O-][N+](=O)c(c(ccc1)C)c1</chem>	000088-72-2	2-Methylnitrobenzene	3.91 ^a	-
61	<chem>c1c([N+](=O)[O-])cc(C)cc1</chem>	000099-08-1	3-Methylnitrobenzene	3.74 ^a	-
62	<chem>c1c([N+](=O)[O-])ccc(C)c1</chem>	000099-99-0	4-Methylnitrobenzene	3.90 ^a	3.74 ^b
63	<chem>[O-][N+](=O)c(c(ccc1)Cl)c1</chem>	000088-73-3	2-Chloronitrobenzene	3.97 ^a	3.94 ^b
64	<chem>c1cc([N+](=O)[O-])cc(Cl)c1</chem>	000121-73-3	3-Chloronitrobenzene	4.05 ^a	3.95 ^b
65	<chem>c1c([N+](=O)[O-])ccc(Cl)c1</chem>	000100-00-5	4-Chloronitrobenzene	3.94 ^a	4.01 ^b
66	<chem>c1c([N+](=O)[O-])cc(Br)cc1</chem>	000585-79-5	3-Bromonitrobenzene	4.41 ^a	4.32 ^b
67	<chem>c1c([N+](=O)[O-])ccc(Br)c1</chem>	000586-78-7	4-Bromonitrobenzene	4.68 ^a	3.88 ^b

68	<chem>c1cc([N+](=O)[O-])cc(Cl)c1F</chem>	000350-30-1	3-Chloro-4-fluoronitrobenzene	3.68 ^a	
69	<chem>c1c([N+](=O)[O-])c(Cl)cc(Cl)c1</chem>	000611-06-3	2,4-Dichloronitrobenzene	5.58 ^a	
70	<chem>c1c(Cl)c([N+](=O)[O-])cc(Cl)c1</chem>	000089-61-2	2,5-Dichloronitrobenzene	4.22 ^a	4.31 ^b
71	<chem>c1c([N+](=O)[O-])cc(Cl)c(Cl)c1</chem>	000099-54-7	3,4-Dichloronitrobenzene	4.12	4.52
72	<chem>c1c([N+](=O)[O-])c(N)ccc1</chem>	000088-74-4	2-Nitroaniline	3.71 ^a	3.33 ^b
73	<chem>c1c([N+](=O)[O-])cc(N)cc1</chem>	000099-09-2	3-Nitroaniline	3.77	3.48
74	<chem>c1c([N+](=O)[O-])ccc(N)c1</chem>	000100-01-6	4-Nitroaniline	3.70 ^a	3.40 ^b
75	<chem>c1cc([N+](=O)[O-])cc(Cl)c1N</chem>	000121-87-9	2-Chloro-4-nitroaniline	3.99 ^a	-
76	<chem>[O-][N+](=O)c(c(O)ccc1)c1</chem>	000088-75-5	2-Nitrophenol	3.53 ^a	3.51 ^b
77	<chem>[O-][N+](=O)c(cccc1O)c1</chem>	000554-84-7	3-Nitrophenol	3.34 ^a	3.75 ^b
78	<chem>[O-][N+](=O)c(ccc(O)c1)c1</chem>	000100-02-7	4-Nitrophenol	3.70 ^a	3.57 ^b
79	<chem>c1c([N+](=O)[O-])c(OC)ccc1</chem>	000091-23-6	2-Nitroanisole	3.50 ^a	3.44 ^b
80	<chem>c1c([N+](=O)[O-])cc(OC)cc1</chem>	000555-03-3	3-Nitroanisole	4.12 ^a	3.71 ^b
81	<chem>c1c([N+](=O)[O-])ccc(OC)c1</chem>	000100-17-4	4-Nitroanisole	-	3.65 ^b
82	<chem>c1cc([N+](=O)[O-])c2ccccc2c1</chem>	000086-57-7	1-Nitronaphthalene	4.79 ^a	-
83	<chem>c1c([N+](=O)[O-])ccc(C=O)c1</chem>	000555-16-8	4-Nitrobenzaldehyde	4.28 ^a	-
84	<chem>c1cc([N+](=O)[O-])c([N+](=O)[O-])cc1</chem>	000528-29-0	1,2-Dinitrobenzene	6.03 ^a	5.04 ^b
85	<chem>c1cc([N+](=O)[O-])cc([N+](=O)[O-])c1</chem>	000099-65-0	1,3-Dinitrobenzene	4.93 ^a	4.85 ^b
86	<chem>c1c([N+](=O)[O-])ccc([N+](=O)[O-])c1</chem>	000100-25-4	1,4-Dinitrobenzene	5.84 ^a	4.96 ^b
87	<chem>c1c([N+](=O)[O-])cc([N+](=O)[O-])c(C)c1</chem>	000121-14-2	2,4-Dinitrotoluene	4.64 ^a	4.52 ^b
88	<chem>c1c([N+](=O)[O-])c(C)c([N+](=O)[O-])cc1</chem>	000606-20-2	2,6-Dinitrotoluene	4.27	4.06
89	<chem>c1c([N+](=O)[O-])cc([N+](=O)[O-])c(Cl)c1</chem>	000097-00-7	2,4-Dinitrochlorobenzene	5.58 ^a	5.52 ^b
90	<chem>c1cc([N+](=O)[O-])cc([N+](=O)[O-])c1Br</chem>	000584-48-5	2,4-Dinitrobromobenzene	5.00 ^a	-
91	<chem>c1c(N)c([N+](=O)[O-])cc([N+](=O)[O-])c1</chem>	000097-02-9	2,4-Dinitroaniline	4.16 ^a	4.68 ^b
92	<chem>[O-][N+](=O)c(ccc(O)c1[N+](=O)[O-])c1</chem>	000051-28-5	2,4-Dinitrophenol	4.09 ^a	4.16 ^b
93	<chem>c1cc(C=O)ccc1Cl</chem>	000104-88-1	4-Chlorobenzaldehyde	4.15 ^a	-
94	<chem>c1c(C=O)cccc1Cl</chem>	000587-04-2	3-Chlorobenzaldehyde	4.00 ^a	-
95	<chem>O=Cc1ccc(Cl)c(Cl)c1</chem>	006287-38-3	3,4-Dichlorobenzaldehyde	4.68 ^a	-
96	<chem>N#Cc1ccc(Cl)c(Cl)c1</chem>	006574-99-8	3,4-Dichlorobenzonitrile	4.22 ^a	-

97	<chem>N#Cc1ccc(Cl)cc1</chem>	000623-03-0	4-Chlorobenzonitrile	4.20 ^a	-
98	<chem>N#CCc1ccc(Cl)cc1</chem>	000140-53-4	4-Chlorobenzyl cyanide	4.73 ^a	-
99	<chem>N#CCc1c(Cl)cccc1</chem>	002856-63-5	2-Chlorobenzyl cyanide	4.26 ^a	-
100	<chem>c1cc(CCl)ccc1Cl</chem>	000104-83-6	4-Chlorobenzyl chloride	5.01 ^a	-
101	<chem>c1ccccc1C(=O)O</chem>	000065-85-0	Benzoic acid	4.09 ^a	-
102	<chem>c1cc(Cl)ccc1C(=O)O</chem>	000074-11-3	4-Chlorobenzoic acid	4.39 ^a	-
103	<chem>c1ccc(Cl)cc1C(=O)O</chem>	000535-80-8	3-Chlorobenzoic acid	4.32 ^a	-
104	<chem>c1cccc(Cl)c1C(=O)O</chem>	000118-91-2	2-Chlorobenzoic acid	4.17 ^a	-
105	<chem>c1cc(Br)ccc1C(=O)O</chem>	000586-76-5	4-Bromobenzoic acid	4.83 ^a	-
106	<chem>c1ccc(Br)cc1C(=O)O</chem>	000585-76-2	3-Bromobenzoic acid	4.66 ^a	-
107	<chem>c1cc(F)ccc1C(=O)O</chem>	000456-22-4	4-Fluorobenzoic acid	4.39 ^a	-
108	<chem>c1cc(N)ccc1C(=O)O</chem>	000150-13-0	4-Aminobenzoic acid	4.00 ^a	-
109	<chem>c1ccc(N)cc1C(=O)O</chem>	000099-05-8	3-Aminobenzoic acid	3.87 ^a	-
110	<chem>c1cccc(N)c1C(=O)O</chem>	000118-92-3	2-Aminobenzoic acid	4.00 ^a	-
111	<chem>c1ccc(C(=O)O)cc1C(=O)O</chem>	000121-91-5	3-Phthalic acid	4.23 ^a	-
112	<chem>c1cccc(C(=O)O)c1C(=O)O</chem>	000088-99-3	2-Phthalic acid	4.40 ^a	-

^achemical not included in algae(*P. subcapitata*) data; ^bchemical not included in algae(*P. subcapitata*) data