

Supplementary Information

Modeling Toxicity of Chemical Pesticides in Multiple Test Species Using Local and Global QSTR Approaches

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Table S1: Data set used in QSTR modeling

S.No.	Chemical name	CAS No.	Taxonomic name	nta	TPSA	PEOEVSA13	LogP	Hy	Aweight	J	pEC ₅₀ / pLC ₅₀ (mM)
1	(S)-Dimethenamid	163515-14-8	Daphnia magna	35	29.540	0.000	2.972	-2.885	15.156	2.807	1.361
2	1,2-Benzenedicarboxaldehyde	643-79-8	Daphnia magna	16	34.140	0.000	1.312	-2.658	12.809	2.340	3.188
3	1,2-Benzisothiazolin-3-one	2634-33-5	Daphnia magna	15	32.860	0.000	1.108	-2.325	14.615	2.015	2.138
4	1,2-Benzisothiazolin-3-one, 2-butyl	4299-07-4	Daphnia magna	27	22.000	0.000	2.863	-2.991	13.871	1.889	3.330
5	1,3 Dichloropropene	542-75-6	Daphnia magna	9	0.000	0.000	1.978	-1.393	21.388	2.191	3.091
6	1,3,5-Triethylhexahydro-s-triazine, VancideTH	7779-27-3	Daphnia magna	33	9.720	0.000	0.838	-2.689	12.510	2.405	1.049
7	1,4-Bis(bromoacetoxy)-2-butene (BBAB)	20679-58-7	Daphnia magna	24	52.600	11.939	1.419	-2.176	22.849	3.060	3.372
8	2-(Hydroxymethylamino)ethanol	34375-28-5	Daphnia magna	15	52.490	0.000	-1.482	-1.292	13.673	2.339	0.558
9	2,4-D 2-EHE Selective Weed Killer	1928-43-4	Daphnia magna	43	35.530	5.969	5.609	-3.347	14.813	2.554	2.824

10	2,4-D Acid	94-75-7	Daphnia magna	19	46.530	5.969	2.457	-2.277	16.538	2.254	0.947
11	2,4-D Butoxyethanol Ester	1929-73-3	Daphnia magna	38	44.760	5.969	3.732	-3.025	15.153	2.004	2.276
12	2,4-D Isooctyl Ester	25168-26-7	Daphnia magna	43	35.530	5.969	5.132	-3.347	14.813	1.994	3.790
13	2,4-D Isopropyl Ester	94-11-1	Daphnia magna	28	35.530	5.969	3.324	-2.750	15.689	2.214	2.005
14	2,4-D Propylene Glycol B.E. Ester	1320-18-9	Daphnia magna	41	44.760	5.969	4.121	-3.137	15.003	2.088	2.446
15	2,4-DB Acid	94-82-6	Daphnia magna	25	46.530	5.969	3.237	-2.605	15.934	2.101	0.993
16	2,4-DP 2-Butoxyethyl Ester Weedone formula	53404-31-2	Daphnia magna	41	44.760	5.969	4.121	-3.137	15.003	2.139	4.729
17	2-Benzyl-4-chlorophenol (Nipacide BCP)	120-32-1	Daphnia magna	26	20.230	0.000	3.636	-3.386	13.840	1.802	2.569
18	2-Bromo-4'-hydroxyacetophenone (BHAP)	2491-38-5	Daphnia magna	18	37.300	0.000	1.970	-2.516	18.908	2.268	1.500
19	2-EEEBC (Debacarb)	62732-91-6	Daphnia magna	40	85.470	6.093	1.683	-2.928	13.056	1.486	-0.964
20	2-Hydroxyacetophenone	118-93-4	Daphnia magna	18	37.300	0.000	0.862	-2.658	12.809	2.240	0.456
21	2-Hydroxyethyl octyl sulfide MGK 874 repellent	3547-33-9	Daphnia magna	34	20.230	0.000	3.072	-2.987	14.015	2.727	2.711
22	2-Hydroxypropyl methanethiosulfonate(HPMETS)	30388-01-3	Daphnia magna	19	54.370	0.000	0.060	-1.409	17.797	3.281	1.152
23	2-Methyl Benzisothiazolone(MBIT)	2527-66-4	Daphnia magna	18	22.000	0.000	1.600	-2.516	14.378	2.054	2.254
24	3,5 Dimethyl-1-(hydroxymethyl)pyrazole	85264-33-1	Daphnia magna	19	38.050	0.000	0.450	-2.113	12.898	2.379	0.600
25	3-Iodo-2-propynyl butyl carbamate (IPBC)	55406-53-6	Daphnia magna	24	38.330	6.093	1.909	-2.390	22.416	3.042	3.245
26	4,4-Dimethyloxazolidine	51200-87-4	Daphnia magna	18	21.260	0.000	0.342	-2.005	12.866	2.400	0.352
27	4,5-Dichloro-1,2-dithiol-3-one(Dearborn 1235)	1192-52-5	Daphnia magna	10	17.070	0.000	0.718	-1.125	23.384	2.436	1.403
28	4,5-Dichloro-2-n-octyl-3(2H)-isothiazolone	64359-81-5	Daphnia magna	34	20.310	0.000	3.709	-2.750	16.569	2.051	4.733
29	4-Chloro-3,5-xyleneol (Ottasept))	88-04-0	Daphnia magna	19	20.230	0.000	2.662	-2.658	14.754	2.487	1.763
30	4-Chloro-3-cresol	59-50-7	Daphnia magna	16	20.230	0.000	2.354	-2.465	15.059	2.346	1.792
31	Acephate	30560-19-1	Daphnia magna	20	55.400	6.721	1.240	-1.329	17.309	3.803	2.149
32	Acequinocyl (AKM-05 degradate)	57960-19-7	Daphnia magna	60	60.440	5.969	6.194	-4.121	12.581	1.738	5.205

33	Acetamiprid IM 1 5 metabolite (CAS 125-147)	135410-20-7	Daphnia magna	26	52.280	0.000	2.066	-2.605	14.106	2.221	0.959
34	Acetochlor WF2061 formulation	34256-82-1	Daphnia magna	38	29.540	0.000	3.123	-3.243	13.867	2.775	1.574
35	Acibenzolar-s-methyl	135158-54-2	Daphnia magna	19	42.850	0.000	2.195	-2.277	15.710	2.008	1.860
36	Alachlor	15972-60-8	Daphnia magna	38	29.540	0.000	2.987	-3.243	13.867	2.859	1.544
37	Aldicarb	116-06-3	Daphnia magna	26	50.690	6.093	1.470	-2.091	14.680	3.423	2.666
38	Aldoxycarb	1646-88-4	Daphnia magna	28	84.830	6.093	0.151	-1.904	14.868	3.889	2.900
39	Alpha-cypermethrin BAS 310 40 I formulation	67375-30-8	Daphnia magna	47	59.320	5.969	6.178	-3.777	14.184	1.507	5.813
40	Ametryn	834-12-8	Daphnia magna	32	62.730	0.000	1.846	-2.344	14.013	2.429	0.909
41	Amicarbazone	129909-90-6	Daphnia magna	36	94.940	11.721	0.238	-2.404	13.067	2.668	0.772
42	Aminocarb	2032-59-9	Daphnia magna	31	41.570	6.093	1.779	-2.865	12.809	2.368	4.620
43	Aminocyclopyrachlor methyl ester	858954-83-3	Daphnia magna	25	78.100	5.969	1.376	-2.344	14.505	1.998	1.029
44	Amitraz	33089-61-1	Daphnia magna	45	27.960	0.000	4.872	-3.851	12.283	1.624	1.939
45	Amitrole	61-82-5	Daphnia magna	10	67.590	0.000	-1.095	-0.862	13.342	2.184	1.086
46	Anilazine	101-05-3	Daphnia magna	21	50.700	0.000	3.575	-2.250	16.905	1.829	2.463
47	Aspon (Ortho Sod-Cancelled in U.S.)	3244-90-4	Daphnia magna	51	46.150	140.999	5.924	-2.510	16.677	4.805	5.758
48	Asulam	3337-71-1	Daphnia magna	25	98.490	6.093	0.313	-2.084	14.678	2.457	0.931
49	Atrazine	1912-24-9	Daphnia magna	28	62.730	0.000	1.777	-2.176	14.398	2.368	1.495
50	Azadirachtin	108168-76-9	Daphnia magna	95	212.040	23.877	0.942	-3.893	13.262	1.718	1.889
51	Azinphos-methyl	86-50-0	Daphnia magna	32	66.240	119.410	2.382	-2.236	16.065	1.873	5.448
52	Azoxystrobin	131860-33-8	Daphnia magna	47	103.560	5.969	4.093	-3.598	12.875	1.562	3.192
53	BCDM Hydantoin, 1-bromo-3- chloro-5,5-dimethyl	16079-88-2	Daphnia magna	17	40.620	6.031	1.493	-1.572	21.402	2.867	2.650
54	Bendiocarb	22781-23-3	Daphnia magna	29	56.790	6.093	1.912	-2.750	13.133	1.985	3.883
55	Benfluralin Balan EC formulation	1861-40-1	Daphnia magna	39	89.520	6.176	4.148	-2.557	13.876	3.103	2.186
56	Benomyl 50WP formulation	17804-35-2	Daphnia magna	39	85.250	12.124	2.572	-2.928	12.961	1.989	3.329
57	Bensulide	741-58-2	Daphnia magna	47	64.630	0.000	4.423	-2.753	16.232	2.210	2.836
58	Bentazon	50723-80-3	Daphnia magna	28	66.480	10.209	1.207	-2.500	14.262	2.206	0.575
59	Benzyl bromoacetate	5437-45-6	Daphnia magna	21	26.300	5.969	2.125	-2.689	18.333	2.046	2.998
60	Bethoxazin BTCN metabolite (Canceled in U.S.)	163269-30-5	Daphnia magna	26	41.490	0.000	2.940	-2.750	15.141	1.627	2.196

61	Bifenazate	149877-41-8	Daphnia magna	42	59.590	6.093	3.824	-3.446	12.736	1.822	2.779
62	Bifenthrin	82657-04-3	Daphnia magna	51	26.300	12.146	6.662	-3.853	13.817	1.497	5.422
63	Biobor JF (7.2% as boron)	2665-13-6	Daphnia magna	44	55.380	14.642	1.419	-2.593	13.087	1.562	-0.407
64	Bioresmethrin Bis (3-aminopropyl)dodecylamine)	28434-01-7	Daphnia magna	51	39.440	5.969	5.152	-4.087	12.490	1.361	5.626
65	Lonzabac 12	2372-82-9	Daphnia magna	62	55.280	0.000	3.907	-3.765	12.296	3.352	3.613
66	Bis (trichloromethyl) sulfone	3064-70-8	Daphnia magna	11	34.140	0.000	3.057	-0.629	27.346	4.748	3.240
67	Bitertanol	55179-31-2	Daphnia magna	48	60.170	0.000	3.930	-3.715	12.570	1.533	1.856
68	Boscalid	188425-85-6	Daphnia magna	35	43.200	0.000	4.258	-3.540	14.396	1.993	1.809
69	Brodifacoum	56073-10-0	Daphnia magna	58	50.440	5.626	7.790	-4.543	14.293	1.136	2.728
70	Bromacil	314-40-9	Daphnia magna	27	54.860	5.690	1.097	-2.448	17.715	2.732	0.334
71	Bromadiolone	28772-56-7	Daphnia magna	58	70.670	5.626	7.184	-4.397	14.407	1.223	3.342
72	Bromethalin	63333-35-7	Daphnia magna	34	89.520	6.176	6.577	-2.465	21.144	2.380	5.465
73	Bromonitrostyrene	7166-19-0	Daphnia magna	18	43.140	4.606	2.657	-2.390	18.500	2.195	3.978
74	Bromoxynil AXF 1240 formulation	1689-84-5	Daphnia magna	14	44.020	0.000	2.789	-2.201	24.899	2.474	0.573
75	Bromoxynil butyrate	3861-41-4	Daphnia magna	25	50.090	5.969	3.789	-2.750	21.121	2.463	3.239
76	Bromoxynil heptanoate	56634-95-8	Daphnia magna	34	50.090	5.969	4.959	-3.130	19.682	2.300	4.099
77	Bromoxynil octanoate	1689-99-2	Daphnia magna	37	50.090	5.969	5.349	-3.241	19.299	2.244	3.549
78	Bromuconazole (EXP 10064)	116255-48-2	Daphnia magna	32	39.940	0.000	3.664	-2.809	18.249	1.744	3.647
79	Bronopol Butoxypolypropylene glycol (Stabilene repellent)	52-51-7	Daphnia magna	15	83.600	4.448	-0.661	-1.057	21.549	3.919	2.097
80		9003-13-8	Daphnia magna	35	38.690	0.000	1.589	-2.846	12.931	3.148	0.302
81	Butralin	33629-47-9	Daphnia magna	42	98.310	0.000	4.011	-2.928	13.056	3.009	3.391
82	Butylate	2008-41-5	Daphnia magna	34	20.310	0.000	3.372	-2.846	14.014	3.722	1.233
83	Cadusafos	95465-99-9	Daphnia magna	38	26.300	5.773	5.194	-2.605	16.481	4.293	5.172
84	Captafol (Cancelled in U.S.)	2939-80-2	Daphnia magna	27	37.380	0.000	3.521	-2.317	18.889	2.089	2.006
85	Captan	133-06-2	Daphnia magna	24	37.380	0.000	2.914	-2.250	18.283	2.087	1.554
86	Carbaryl	63-25-2	Daphnia magna	26	38.330	6.093	2.558	-3.126	12.676	1.911	4.861
87	Carbendazim	10605-21-7	Daphnia magna	23	67.010	6.093	1.259	-2.448	13.008	1.805	3.240
88	Carbofuran	1563-66-2	Daphnia magna	31	47.560	6.093	2.118	-3.000	12.883	1.985	3.882
89	Carboxin	5234-68-4	Daphnia magna	29	38.330	0.000	2.620	-3.000	13.888	1.784	0.445

90	Chlorantraniliprole 20 SC formulation	500008-45-7	Daphnia magna	42	81.070	6.093	4.862	-3.090	16.751	1.593	4.833
91	Chlorethoxyfos	54593-83-8	Daphnia magna	27	27.690	115.786	4.619	-1.563	21.661	4.397	5.914
92	Chlorfenapyr	122453-73-0	Daphnia magna	34	37.950	6.176	5.455	-2.950	17.240	2.261	4.718
93	Chlorflurenol methyl ester	37339-61-0	Daphnia magna	30	46.530	5.969	2.729	-3.354	13.874	1.945	1.564
94	Chloroneb	2675-77-6	Daphnia magna	20	18.460	0.000	3.011	-2.390	16.583	2.491	1.524
95	Chlorophacinone	3691-35-8	Daphnia magna	42	51.210	0.000	4.736	-4.050	13.322	1.545	2.944
96	Chloropicrin	76-06-2	Daphnia magna	7	43.140	3.916	1.591	-0.401	23.482	3.541	3.137
97	Chlorothalonil(Degradate)	1897-45-6	Daphnia magna	14	47.580	0.000	4.044	-2.176	18.994	2.824	1.010
98	Chlorpropham	101-21-3	Daphnia magna	26	38.330	6.093	3.297	-2.720	14.398	2.214	1.762
99	Chlorpyrifos	2921-88-2	Daphnia magna	30	40.580	126.958	5.101	-2.085	18.861	2.622	6.545
100	Chlorpyrifos methyl	5598-13-0	Daphnia magna	24	40.580	114.116	4.321	-1.750	19.718	2.594	5.463
101	Chlorsulfuron	64902-72-3	Daphnia magna	35	114.200	16.240	0.101	-2.360	15.030	2.120	-0.015
102	Chlorthal dimethyl (DCPA or Dacthal)	1861-32-1	Daphnia magna	24	52.600	11.939	3.873	-2.317	18.107	2.949	1.134
103	Chromic acid	7738-94-5	Daphnia magna	7	80.260	31.045	-1.354	0.000	23.198	3.024	2.191
104	Cinnamaldehyde	104-55-2	Daphnia magna	18	17.070	0.000	1.899	-2.990	12.410	2.017	1.273
105	Clethodim	99129-21-2	Daphnia magna	49	58.890	0.000	4.844	-3.344	14.509	2.502	1.251
106	Clomazone	81777-89-1	Daphnia magna	30	29.540	0.000	2.640	-3.000	14.099	1.899	1.664
107	Coumaphos	56-72-4	Daphnia magna	39	57.900	138.892	4.814	-2.838	15.757	1.961	6.276
108	Cyanamide (Alzodef)	420-04-2	Daphnia magna	5	49.810	0.000	-0.574	-0.528	13.342	1.633	0.798
109	Cyanazine	21725-46-2	Daphnia magna	29	86.520	0.000	1.671	-2.250	14.225	2.469	0.758
110	Cyantraniliprole WG Cyazofamid (400 SC formulation)	736994-63-1	Daphnia magna	43	112.700	0.000	3.475	-3.183	15.848	1.709	4.910
111	Cycloate	120116-88-3	Daphnia magna	34	78.990	10.209	2.038	-2.719	14.842	2.231	3.313
112	Cyflufenamid 149-F1 metabolite	1134-23-2	Daphnia magna	35	20.310	0.000	3.514	-2.991	13.871	2.415	0.953
113	Cyfluthrin (Tempo 2EC Formulation)	180409-60-3	Daphnia magna	46	50.690	6.176	4.431	-3.350	13.628	1.679	1.457
114	Cyhalothrin	68359-37-5	Daphnia magna	47	59.320	5.969	6.317	-3.685	14.350	1.544	7.240
115	Cyhexatin	68085-85-8	Daphnia magna	50	59.320	12.146	6.544	-3.676	13.894	1.521	6.073
116	Cymoxanil	13121-70-5	Daphnia magna	54	20.230	130.349	5.927	-3.890	17.545	1.791	6.355
117	Cypermethrin Beta	57966-95-7	Daphnia magna	24	103.580	6.031	-0.642	-1.904	13.436	3.829	2.394
118		52315-07-8	Daphnia magna	47	59.320	5.969	6.178	-3.777	14.184	1.507	5.996

119	Cyphenothrin	39515-40-7	Daphnia magna	53	59.320	5.969	5.825	-4.121	12.510	1.507	5.941
120	Cyproconazole	94361-06-5	Daphnia magna	38	50.940	0.000	2.865	-3.241	13.682	1.705	1.050
121	Cyprodinil	121552-61-2	Daphnia magna	32	37.810	0.000	3.406	-3.366	12.363	1.503	3.848
122	Daminozide	1596-84-5	Daphnia magna	23	69.640	5.969	-0.556	-1.887	13.462	3.293	0.211
123	Dazomet	533-74-4	Daphnia magna	19	6.480	0.000	0.797	-1.761	16.911	2.346	2.692
124	DBDMH Glybrom formulation	77-48-5	Daphnia magna	17	40.620	6.031	1.649	-1.572	25.443	2.867	2.532
125	DBNPA	10222-01-2	Daphnia magna	10	66.880	0.000	0.481	-1.125	29.982	3.708	2.449
126	DCDMH (Dantochlor Formulation)	118-52-5	Daphnia magna	17	40.620	6.031	1.337	-1.572	17.361	2.867	2.622
127	DDT (Cancelled in U.S.)	50-29-3	Daphnia magna	28	0.000	0.000	6.496	-3.130	18.180	2.037	4.878
128	Decanol (Alfol 810 alcohol)	112-30-1	Daphnia magna	33	20.230	0.000	3.119	-3.145	12.374	2.691	1.386
129	Deltamethrin	52918-63-5	Daphnia magna	47	59.320	5.969	6.490	-3.777	17.359	1.507	6.662
130	Desmedipham	13684-56-5	Daphnia magna	38	76.660	12.186	3.866	-3.243	12.918	1.673	2.203
131	Diazinon	333-41-5	Daphnia magna	41	53.470	120.148	3.968	-2.683	14.904	2.617	5.766
132	Diazolidinylurea (Integra 22)	78491-02-8	Daphnia magna	19	70.390	6.031	-1.568	-1.409	13.341	2.113	0.351
133	Dibromodicyanobutane	35691-65-7	Daphnia magna	16	47.580	0.000	2.546	-1.993	25.989	3.971	2.082
134	Dicamba	1918-00-9	Daphnia magna	19	46.530	5.969	2.700	-2.277	16.538	2.709	0.300
135	Dichlobenil	1194-65-6	Daphnia magna	13	23.790	0.000	2.865	-2.325	16.899	2.450	1.443
136	Dichlormid	37764-25-3	Daphnia magna	23	20.310	0.000	1.991	-2.390	16.417	3.894	0.169
137	Dichlorprop (2,4-DP) Weedone formulation	120-36-5	Daphnia magna	22	46.530	5.969	2.845	-2.448	16.214	2.371	4.647
138	Dichlorprop P (2,4-DP-p) Dichlorvos in Muscalure Z-9 formulation	15165-67-0	Daphnia magna	22	46.530	5.969	2.845	-2.448	16.214	2.371	-0.375
139	Diclofop-methyl	62-73-7	Daphnia magna	18	44.760	7.823	2.680	-1.258	19.447	3.686	2.311
140	Dicloran (DCNA)	51338-27-3	Daphnia magna	36	44.760	5.969	4.726	-3.243	14.867	1.687	3.171
141	Diclosulam	99-30-9	Daphnia magna	16	69.160	0.000	2.484	-1.792	16.915	2.533	2.000
142	Dicrotophos	145701-21-9	Daphnia magna	36	86.450	6.010	2.943	-2.601	15.766	1.665	0.750
143	Dienochlor	141-66-2	Daphnia magna	31	65.070	7.823	1.396	-2.084	14.738	4.068	4.271
144	Diethyl toluamide (DEET)	2227-17-0	Daphnia magna	20	0.000	0.000	7.726	-2.161	23.732	2.532	2.597
145	Difenoconazole	134-62-3	Daphnia magna	31	20.310	0.000	2.477	-3.263	12.438	2.449	0.407
146	Difethialone	119446-68-3	Daphnia magna	44	58.400	0.000	4.666	-3.346	14.412	1.351	2.722
147	Diflubenzuron	104653-34-1	Daphnia magna	58	37.300	0.000	8.259	-4.543	14.752	1.136	5.089
148		35367-38-5	Daphnia magna	30	58.200	6.031	3.580	-2.928	14.363	1.767	5.316

149	Diiodomethyl p-tolyl sulfone (Amical 48)	20018-09-1	Daphnia magna	21	34.140	0.000	2.922	-2.277	31.843	2.524	3.774
150	Dimethenamid	87674-68-8	Daphnia magna	35	29.540	0.000	2.972	-2.885	15.156	2.807	1.236
151	Dimethepin (Harvade 25F formulation)	55290-64-7	Daphnia magna	22	68.280	0.000	0.081	-1.792	16.683	2.799	1.503
152	Dimethyl disulfide	624-92-0	Daphnia magna	10	0.000	0.000	1.627	-1.000	22.039	1.975	1.767
153	Dinitramine	29091-05-2	Daphnia magna	35	115.540	11.864	2.950	-2.230	14.052	3.268	2.394
154	Dinocap	39300-45-3	Daphnia magna	50	112.580	11.657	5.058	-3.254	13.085	2.895	4.938
155	Diphacinone	82-66-6	Daphnia magna	42	51.210	0.000	4.083	-4.158	12.471	1.551	2.277
156	Diphenamid	957-51-7	Daphnia magna	35	20.310	0.000	2.907	-3.707	12.343	2.045	0.616
157	Diphenylamine	122-39-4	Daphnia magna	24	12.030	0.000	3.430	-3.416	12.165	1.687	2.149
158	Dipropyl isocinchomeronate MGK 326 repellent	136-45-8	Daphnia magna	35	65.490	11.939	2.215	-3.012	13.008	2.227	1.145
159	Disulfoton	298-04-4	Daphnia magna	33	18.460	0.000	4.421	-2.176	18.233	3.303	4.324
160	Dithiopyr Dimension formulation	97886-45-8	Daphnia magna	41	47.030	6.176	5.243	-2.786	15.412	3.432	1.888
161	Diuron Karmex DF Formulation	330-54-1	Daphnia magna	24	32.340	6.031	3.087	-2.448	15.930	2.326	1.443
162	D-Phenothrin (Sumithrin)	26002-80-2	Daphnia magna	52	35.530	5.969	5.761	-4.158	12.471	1.396	4.901
163	DTEA	36362-09-1	Daphnia magna	41	26.020	0.000	3.819	-3.263	13.586	2.785	3.781
164	d-trans-Allethrin	584-79-2	Daphnia magna	48	43.370	5.969	4.002	-3.851	12.555	1.914	4.531
165	Econea (Chlorfenapyr) CL 322, 250 degradate	122454-29-9	Daphnia magna	24	39.580	6.176	4.506	-2.683	18.131	2.076	2.698
166	Endosulfan	115-29-7	Daphnia magna	26	38.360	143.458	4.288	-2.012	21.099	2.109	3.389
167	Endosulfan sulfate metabolite(PC Code 079404)	1031-07-8	Daphnia magna	26	52.600	10.399	3.356	-1.945	20.844	2.094	3.149
168	Endothall	145-73-3	Daphnia magna	23	83.830	11.939	-0.051	-2.277	13.545	2.149	0.758
169	Endrin (Cancelled in U.S.)	72-20-8	Daphnia magna	27	12.530	0.000	4.481	-2.683	19.624	1.758	4.958
170	Esfenvalerate	66230-04-4	Daphnia magna	52	59.320	5.969	6.680	-4.089	13.258	1.539	6.447
171	Ethalfuralin Sonalan EC formulation	55283-68-6	Daphnia magna	37	89.520	6.176	3.924	-2.557	13.876	3.155	4.265
172	Ethephon	16672-87-0	Daphnia magna	13	57.530	7.596	0.403	-0.802	19.778	3.154	0.659
173	Ethion	563-12-2	Daphnia magna	43	36.920	136.803	5.771	-2.012	19.069	4.271	6.837
174	Ethofenprox	80844-07-1	Daphnia magna	56	27.690	0.000	6.372	-4.292	12.438	1.339	5.820
175	Ethofumesate	26225-79-6	Daphnia magna	37	61.830	10.118	2.058	-2.906	14.116	2.023	0.651
176	Ethoprop	13194-48-4	Daphnia magna	32	26.300	5.773	4.417	-2.277	17.169	3.835	3.753

177	Ethoxyquin Ethyl N,N-dipropylthiocarbamate (EPTC)	91-53-2	Daphnia magna	35	21.260	0.000	3.693	-3.500	12.385	1.983	2.036
178	Ethylenethiourea	759-94-4	Daphnia magna	31	20.310	0.000	2.982	-2.689	14.181	3.721	1.128
179	Etoxazole	96-45-7	Daphnia magna	12	24.060	0.000	-0.536	-1.292	16.019	2.184	0.580
180	Etridiazole metabolite(T-03)	153233-91-1	Daphnia magna	49	30.820	0.000	5.179	-3.797	12.932	1.631	4.704
181	Famoxadone	2593-15-9	Daphnia magna	17	35.010	0.000	2.764	-1.494	20.208	2.352	2.352
182	Farnesol	131807-57-3	Daphnia magna	46	67.870	6.093	4.700	-3.777	12.723	1.294	4.501
183	Fenamidone(RPA413255 s- enantiomer)	4602-84-0	Daphnia magna	42	20.230	0.000	4.398	-3.750	12.260	3.324	2.005
184	Fenamiphos Nemacur 3 formulation	161326-34-7	Daphnia magna	39	44.700	0.000	3.490	-3.446	13.376	1.688	1.507
185	Fenarimol	22224-92-6	Daphnia magna	41	47.560	7.746	4.238	-2.906	14.799	2.550	5.368
186	Fenazaquin	60168-88-9	Daphnia magna	34	46.010	0.000	4.068	-3.446	14.505	1.827	1.688
187	Fenbutatin oxide	120928-09-8	Daphnia magna	45	35.010	0.000	4.549	-3.934	12.358	1.366	4.738
188	Fenhexamid	114369-43-6	Daphnia magna	41	54.500	0.000	4.026	-3.630	13.320	1.623	2.166
189	Fenitrothion	13356-08-6	Daphnia magna	141	9.230	396.560	16.761	-5.693	15.462	1.578	4.531
190	Fenoxaprop-ethyl	126833-17-8	Daphnia magna	36	49.330	0.000	4.608	-3.130	15.003	1.925	0.459
191	Fenoxaprop-P metabolite	122-14-5	Daphnia magna	30	70.830	104.345	3.182	-2.164	15.597	2.497	5.081
192	Fenoxycarb	66441-23-4	Daphnia magna	41	70.790	12.046	4.604	-3.344	13.826	1.356	2.056
193	Fenpropathrin	71283-80-2	Daphnia magna	41	70.790	12.046	4.604	-3.344	13.826	1.356	0.458
194	Fenpropimorph	72490-01-8	Daphnia magna	41	56.790	6.093	3.604	-3.446	12.827	1.495	2.877
195	Fenpyrazamine	39515-41-8	Daphnia magna	49	59.320	5.969	5.269	-3.977	12.548	1.521	5.819
196	Fenpyroximate FujiMite 5EC	67564-91-4	Daphnia magna	55	12.470	0.000	4.272	-4.054	12.283	1.706	2.106
197	Fenthion	473798-59-3	Daphnia magna	44	70.020	5.239	3.676	-3.344	13.490	2.205	1.780
198	Fenvalerate	134098-61-6	Daphnia magna	58	74.940	5.969	5.027	-3.836	12.719	1.340	5.421
199	Fipronil MB 46136 metabolite	55-38-9	Daphnia magna	32	27.690	106.534	3.996	-2.500	16.451	2.457	4.729
200	Flazasulfuron DTPU Degradate	51630-58-1	Daphnia magna	52	59.320	5.969	6.680	-4.089	13.258	1.539	6.924
201	Fluazifop-butyl (PP009)	120068-37-3	Daphnia magna	31	87.530	11.685	4.877	-2.169	16.658	2.209	4.178
202	Fluazifop-p-butyl RS 14:1 methanol prepartion	104040-78-0	Daphnia magna	39	123.430	12.207	-0.236	-2.289	14.638	2.164	0.390
203	Fluazifop-p-butyl RS 14:1 methanol prepartion	69806-50-4	Daphnia magna	47	57.650	12.146	5.003	-3.346	13.452	1.614	1.804
204	Fluazifop-p-butyl RS 14:1 methanol prepartion	79241-46-6	Daphnia magna	47	57.650	12.146	5.003	-3.346	13.452	1.614	-0.032
205	Fluazinam	79622-59-6	Daphnia magna	33	111.200	23.727	5.986	-2.178	15.899	2.240	3.412

206	Flubendiamide WG24 formulation	272451-65-7	Daphnia magna	60	84.500	18.021	5.643	-3.176	17.374	1.845	5.482
207	Fluchloralin (uses canceled in U.S.)	33245-39-5	Daphnia magna	36	89.520	6.176	3.977	-2.360	14.895	3.148	2.803
208	Flucythrinate	70124-77-5	Daphnia magna	56	68.550	12.581	6.628	-3.974	12.978	1.521	4.736
209	Fludioxonil(Maxim 4FS)	131341-86-1	Daphnia magna	24	58.040	6.295	2.393	-2.780	13.452	1.752	2.441
210	Flumetsulam	98967-40-9	Daphnia magna	31	89.250	0.000	1.512	-2.432	14.374	1.628	0.107
211	Flumioxazin	103361-09-7	Daphnia magna	41	66.920	0.000	1.928	-3.435	13.047	1.543	1.809
212	Fluometuron	2164-17-2	Daphnia magna	27	32.340	12.207	2.799	-2.500	13.820	2.449	1.370
213	Fluopicolide degradate (2,6- dichlorobenamide)	239110-15-7	Daphnia magna	31	41.990	6.176	4.991	-2.753	16.327	1.815	0.319
214	Fluoxastrobin	361377-29-9	Daphnia magna	48	96.650	0.000	4.565	-3.281	13.835	1.383	2.980
215	Fluridone	59756-60-4	Daphnia magna	38	22.000	6.176	4.738	-3.630	13.134	1.689	2.040
216	Flurprimidol	56425-91-3	Daphnia magna	37	55.240	6.362	3.267	-3.041	13.508	1.989	1.482
217	Flutriafol 125 g/L SC formulation	76674-21-0	Daphnia magna	35	50.940	0.000	2.492	-3.243	13.100	1.762	1.631
218	Fluvalinate	69409-94-5	Daphnia magna	57	71.350	12.146	7.396	-3.810	13.736	1.536	6.099
219	Fluxapyroxad	907204-31-3	Daphnia magna	39	46.920	0.000	4.694	-3.170	13.674	1.649	1.750
220	Folpet	133-07-3	Daphnia magna	20	37.380	0.000	3.259	-2.250	18.283	2.087	2.735
221	Fonofos	944-22-9	Daphnia magna	30	9.230	95.891	4.528	-2.720	16.515	2.369	5.082
222	Forchlorfenuron	68157-60-8	Daphnia magna	27	54.020	6.031	3.379	-2.885	13.977	1.665	1.670
223	Fosthiazate	98886-44-3	Daphnia magna	34	46.610	6.721	3.832	-2.250	16.576	2.695	3.037
224	Furfural	98-01-1	Daphnia magna	11	30.210	0.000	1.092	-2.005	13.150	2.140	0.673
225	Gamma cyhalothrin	76703-62-3	Daphnia magna	50	59.320	12.146	6.544	-3.676	13.894	1.521	7.000
226	Glutaraldehyde	111-30-8	Daphnia magna	15	34.140	0.000	0.554	-2.005	13.150	2.447	2.125
227	Glyphosate N- (phosphonomethyl) glycine	1071-83-6	Daphnia magna	18	106.860	13.565	-1.204	-0.997	16.101	3.205	0.101
228	Grotan	4719-04-4	Daphnia magna	36	70.410	0.000	-2.245	-2.344	13.208	2.400	0.924
229	Halofenozide	112226-61-6	Daphnia magna	42	49.410	0.000	3.926	-3.540	13.551	1.972	1.963
230	Haloxypop acid Hexaconazole JF 9445	69806-34-4	Daphnia magna	35	68.650	12.146	4.398	-2.866	14.609	1.724	0.573
231	formulation - test 1	79983-71-4	Daphnia magna	37	50.940	0.000	3.663	-3.025	14.854	2.034	2.218
232	Hexadecadienol acetate	53042-79-8	Daphnia magna	52	26.300	5.969	5.930	-3.890	12.410	2.924	2.603
233	Hexaflumuron	86479-06-3	Daphnia magna	37	67.430	18.565	5.470	-2.680	15.623	1.863	6.619

234	Hexazinone	51235-04-2	Daphnia magna	38	60.130	11.379	0.513	-2.780	12.898	2.071	0.473
235	Hexythiazox PT-1-9	78587-05-0	Daphnia magna	44	49.410	6.031	4.981	-3.344	14.423	1.563	1.652
236	Hydramethylnon	67485-29-4	Daphnia magna	59	48.780	12.353	6.382	-3.664	13.437	1.446	2.637
237	Hymexazol	10004-44-1	Daphnia magna	12	46.000	0.000	-0.206	-1.604	13.436	2.257	0.507
238	Imazalil	35554-44-0	Daphnia magna	33	27.050	0.000	4.134	-3.130	14.899	1.905	1.973
239	Imazamethabenz	81405-85-8	Daphnia magna	41	67.760	5.969	2.073	-3.347	12.771	2.143	0.117
240	Imazaquin	81335-37-7	Daphnia magna	40	91.650	5.969	2.224	-3.344	12.792	1.766	0.046
241	Imazosulfuron	122548-33-8	Daphnia magna	41	110.800	6.031	0.677	-2.465	14.804	1.702	1.111
242	Imidacloprid	138261-41-3	Daphnia magna	27	85.400	0.000	0.383	-2.164	14.446	1.769	0.477
243	Imiprothrin (Pralle) Indaziflam SC 200 G dual isomer mixture	72963-72-5	Daphnia magna	45	66.920	12.000	1.623	-3.344	12.878	1.839	3.795
244		950782-86-2	Daphnia magna	42	76.720	0.000	3.138	-3.243	12.782	1.633	0.189
245	Indole-3-butyric acid	133-32-4	Daphnia magna	28	53.090	5.969	2.093	-3.126	12.676	1.730	0.552
246	Indoxacarb IN-MP819	173584-44-6	Daphnia magna	53	106.970	24.456	4.093	-3.159	14.186	1.478	3.916
247	Inert Surfadone(LP100)	2687-94-7	Daphnia magna	17	33.020	0.000	1.706	-2.516	13.190	2.374	1.299
248	Ipconazole	125225-28-7	Daphnia magna	47	50.940	0.000	3.588	-3.540	13.464	1.664	2.293
249	Iprodione	36734-19-7	Daphnia magna	34	69.720	12.062	2.880	-2.719	15.098	2.034	3.139
250	Irgarol Isazophos methyl Triumph 4E formulation	28159-98-0	Daphnia magna	36	62.730	0.000	2.378	-2.645	13.778	1.866	1.679
251		42509-83-1	Daphnia magna	30	58.400	104.733	2.791	-1.750	17.037	2.525	5.113
252	Isofenphos metabolite	25311-71-1	Daphnia magna	47	56.790	137.903	4.273	-3.041	14.600	2.751	5.334
253	Isomate C Sex Pheromone	33956-49-9	Daphnia magna	35	20.230	0.000	3.452	-3.416	12.318	2.758	1.814
254	Isopropalin	33820-53-0	Daphnia magna	45	89.520	0.000	4.253	-3.041	13.008	3.082	3.061
255	Kepone (Cancelled in U.S.)	143-50-0	Daphnia magna	21	17.070	0.000	4.823	-2.092	23.364	2.037	3.276
256	Kinoprene	42588-37-4	Daphnia magna	48	26.300	5.969	4.518	-3.890	12.410	3.516	3.442
257	Kresoxim methyl	143390-89-0	Daphnia magna	42	57.120	5.969	2.611	-3.540	12.791	1.975	2.975
258	Lactofen	77501-63-4	Daphnia magna	46	104.970	18.115	5.168	-3.036	14.408	1.966	2.363
259	Lambda-Cyhalothrin	91465-08-6	Daphnia magna	50	59.320	12.146	6.544	-3.676	13.894	1.521	7.051
260	Limonene	138-86-3	Daphnia magna	26	0.000	0.000	3.309	-3.322	12.011	2.260	0.543
261	Linalool	78-70-6	Daphnia magna	29	20.230	0.000	2.670	-3.145	12.374	3.376	0.624
262	Lindane	58-89-9	Daphnia magna	18	0.000	0.000	3.644	-1.792	23.732	2.760	1.664
263	Linuron	330-55-2	Daphnia magna	25	41.570	6.031	3.019	-2.344	15.934	2.330	3.317
264	L-Lactic acid	79-33-4	Daphnia magna	12	57.530	5.969	-0.548	-1.292	14.005	2.993	-0.920

265	Malathion	121-75-5	Daphnia magna	39	71.060	122.751	2.505	-2.236	16.380	4.654	5.519
266	Maleic hydrazide	123-33-1	Daphnia magna	12	65.720	0.000	-1.901	-1.500	13.507	2.192	0.018
267	Mandipropamid	374726-62-2	Daphnia magna	51	56.790	0.000	3.410	-3.853	13.438	1.750	1.764
268	MCPA 2-ethylhexyl ester	29450-45-1	Daphnia magna	46	35.530	5.969	4.787	-3.556	13.697	2.164	3.048
269	MCPA isooctyl ester (Rhonox formula)	26544-20-7	Daphnia magna	46	35.530	5.969	4.787	-3.556	13.697	1.994	3.033
270	Mefenpyr diethyl	135590-91-9	Daphnia magna	42	68.200	11.939	3.444	-3.057	14.796	2.199	1.824
271	Mesotrione(MNBA metabolite)	104206-82-8	Daphnia magna	36	128.490	0.000	1.119	-2.753	14.184	2.134	0.404
272	Metaflumizone 320 I formulation	139968-49-3	Daphnia magna	52	86.510	18.570	6.244	-3.447	13.619	1.505	2.296
273	Metalaxyl Ridomil 2E-G	57837-19-1	Daphnia magna	41	55.840	5.969	1.844	-3.241	12.908	2.950	1.349
274	Metconazole (cis/trans isomers)	125116-23-6	Daphnia magna	44	50.940	0.000	3.342	-3.446	13.530	1.656	1.734
275	Methamidophos	10265-92-6	Daphnia magna	15	52.320	6.721	1.063	-0.802	19.010	3.360	3.735
276	Methidathion	950-37-8	Daphnia magna	28	62.580	106.719	1.904	-1.500	18.203	2.377	4.674
277	Methiocarb	2032-65-7	Daphnia magna	30	38.330	6.093	2.744	-2.865	14.013	2.451	4.074
278	Methomyl	16752-77-5	Daphnia magna	20	50.690	6.093	1.039	-1.661	15.213	3.168	4.266
279	Methoprene	40596-69-8	Daphnia magna	56	35.530	5.969	5.062	-3.851	12.555	3.681	2.543
280	Methoxyfenozide	161050-58-4	Daphnia magna	55	58.640	0.000	4.206	-3.874	12.602	2.093	1.998
281	Methyl anthralinate	134-20-3	Daphnia magna	20	52.320	5.969	1.055	-2.516	12.918	2.402	0.919
282	Methyl chloroform	71-55-6	Daphnia magna	8	0.000	0.000	2.377	-0.929	26.076	3.024	1.076
283	Methyl isothiocyanate	556-61-6	Daphnia magna	7	12.360	0.000	0.719	-1.000	17.524	1.975	2.983
284	Methyl nonyl ketone	112-12-9	Daphnia magna	34	17.070	0.000	3.716	-3.286	12.343	2.817	2.499
285	Methyl parathion	298-00-0	Daphnia magna	27	70.830	97.925	2.874	-2.000	15.821	2.367	6.274
286	Methylene bis(thiocyanate) Slime-trol RX32	6317-18-6	Daphnia magna	9	47.580	0.000	1.372	-1.203	18.312	2.447	1.569
287	Methylisothiazolinone (Kathon OM formulation)	2682-20-4	Daphnia magna	12	22.000	0.000	0.447	-1.604	15.731	2.325	2.806
288	Methylisothiazolinone(Kathon 886 formulation)	26172-55-4	Daphnia magna	12	22.000	0.000	1.100	-1.500	18.196	2.388	2.920
289	Metofluthrin	240494-70-6	Daphnia magna	45	35.530	5.969	4.281	-3.344	13.607	1.937	4.885
290	Metolachlor CGA-51502	51218-45-2	Daphnia magna	41	29.540	0.000	3.164	-3.354	13.770	2.914	1.265
291	Metrafenone CL 4084564 metabolite	220899-03-6	Daphnia magna	46	53.990	0.000	4.331	-3.529	15.524	2.287	0.905
292	Metribuzin	21087-64-9	Daphnia magna	28	73.800	0.000	0.372	-2.176	14.299	2.689	1.710

293	Mexacarbate (Zectran)	315-18-4	Daphnia magna	34	41.570	6.093	2.088	-3.000	12.759	2.518	3.734
294	MGK-264	113-48-4	Daphnia magna	45	37.380	0.000	3.006	-3.674	12.510	1.651	2.078
295	Mirex (Cancelled in U.S.)	2385-85-5	Daphnia magna	22	0.000	0.000	7.664	-2.027	24.798	2.368	2.442
296	Mitin FF	3567-25-7	Daphnia magna	43	104.730	6.031	6.983	-3.036	16.455	1.585	1.742
297	MTI	82633-79-2	Daphnia magna	19	22.000	0.000	0.935	-2.325	14.615	2.091	2.077
298	Myclobutanil	88671-89-0	Daphnia magna	37	54.500	0.000	3.583	-3.241	13.582	2.033	1.419
299	N,N-Methylenebis morpholine metabolite	5625-90-1	Daphnia magna	31	24.940	0.000	-0.392	-2.562	12.932	1.687	0.890
300	N6-Benzyladenine	1214-39-7	Daphnia magna	28	66.490	0.000	1.435	-2.885	12.598	1.465	1.041
301	Naled	300-76-5	Daphnia magna	20	44.760	7.823	3.651	-1.139	28.748	4.254	6.104
302	Naphthalene	91-20-3	Daphnia magna	18	0.000	0.000	2.840	-3.322	12.011	1.925	1.904
303	Naphthaleneacetate acid ethyl ester	2122-70-5	Daphnia magna	30	26.300	5.969	2.945	-3.500	12.509	1.865	0.954
304	Naphthaleneacetic acid	86-87-3	Daphnia magna	24	37.300	5.969	2.467	-3.263	12.581	1.940	0.015
305	Napropamide	15299-99-7	Daphnia magna	41	29.540	0.000	3.476	-3.674	12.510	1.900	1.278
306	Neurolidol	7212-44-4	Daphnia magna	50	58.100	5.690	3.197	-3.777	12.759	1.156	2.237
307	Niclosamide	1420-04-8	Daphnia magna	29	92.470	0.000	3.860	-2.719	15.193	1.860	3.214
308	Nitrapyrin	1929-82-4	Daphnia magna	14	12.890	0.000	3.562	-1.887	20.717	2.461	2.021
309	N-Methyl-2-pyrrolidine N-methylneodecanamide (MNDA)	120-94-5	Daphnia magna	17	3.240	0.000	0.712	-2.154	12.344	2.184	-1.769
310		105726-67-8	Daphnia magna	36	29.100	0.000	2.729	-3.131	12.471	4.418	0.154
311	Nonanoic acid	112-05-0	Daphnia magna	29	37.300	5.969	2.822	-2.830	12.736	2.796	0.217
312	Novaluron 10 EC formulation	116714-46-6	Daphnia magna	41	76.660	24.860	3.087	-2.656	15.114	1.540	5.058
313	Noviflumuron	121451-02-3	Daphnia magna	40	67.430	18.316	6.245	-2.599	15.821	1.974	6.235
314	OBPA	58-36-6	Daphnia magna	45	27.690	179.639	2.826	-4.020	16.762	1.285	5.020
315	Octhilinone	26530-20-1	Daphnia magna	34	20.310	0.000	2.576	-2.991	13.871	1.879	3.300
316	Ortho-phenyl phenol	90-43-7	Daphnia magna	23	20.230	0.000	3.059	-3.416	12.318	1.885	1.831
317	Oryzalin	19044-88-3	Daphnia magna	41	149.680	11.375	1.777	-2.360	14.270	3.148	2.363
318	Oxadiazon	19666-30-9	Daphnia magna	40	57.260	5.756	4.217	-3.041	14.867	2.064	2.814
319	Oxadixyl (canceled in the U.S.)	77732-09-3	Daphnia magna	38	59.080	6.093	1.650	-3.025	13.008	2.196	-0.280
320	Oxamyl	23135-22-0	Daphnia magna	27	71.000	6.093	0.107	-1.904	14.726	3.899	2.669
321	Oxazolidine E	7747-35-5	Daphnia magna	23	21.700	0.000	0.413	-2.325	13.008	2.153	0.533
322	Oxycarboxin	5259-88-1	Daphnia magna	31	72.470	0.000	1.302	-2.780	14.122	1.944	0.588

323	Oxydemeton-methyl	301-12-2	Daphnia magna	29	55.430	6.798	2.487	-1.708	17.782	3.610	3.187
324	Oxyfluorfen	42874-03-3	Daphnia magna	35	61.600	11.864	5.458	-2.866	14.609	1.877	3.655
325	Oxythioquinox	2439-01-2	Daphnia magna	21	42.850	0.000	2.575	-2.605	15.217	1.688	3.291
326	Paclobutrazol	76738-62-0	Daphnia magna	40	50.940	0.000	3.122	-3.241	13.682	1.984	0.947
327	Paranitrophenol	100-02-7	Daphnia magna	15	63.370	0.000	1.300	-1.993	13.407	2.260	1.365
328	Parathion 8E Formulation	56-38-2	Daphnia magna	33	70.830	110.766	3.654	-2.317	15.397	2.418	4.987
329	Pebulate	1114-71-2	Daphnia magna	34	20.310	0.000	3.372	-2.846	14.014	3.632	1.474
330	Pendimethalin	40487-42-1	Daphnia magna	39	98.310	5.687	3.720	-2.809	13.108	2.990	3.002
331	Pentachloronitrobenzene (PCNB)	82-68-8	Daphnia magna	14	43.140	5.687	4.862	-1.632	21.095	2.861	2.584
332	Pentachlorophenol	87-86-5	Daphnia magna	13	20.230	0.000	4.659	-1.792	22.111	2.760	2.295
333	Penthiopyrad 20 SC formulation	183675-82-3	Daphnia magna	44	46.920	6.176	4.902	-3.057	14.136	1.982	3.094
334	Permethrin 3.2 EC	52645-53-1	Daphnia magna	46	35.530	5.969	6.113	-3.797	14.274	1.396	6.414
335	Phenmedipham	13684-63-4	Daphnia magna	38	76.660	12.186	3.784	-3.243	12.918	1.697	1.331
336	Phenthoate (Cidial)	2597-03-7	Daphnia magna	37	44.760	123.194	3.924	-2.683	15.960	2.723	5.227
337	Phosalone	2310-17-0	Daphnia magna	37	53.600	137.193	4.619	-2.510	16.795	1.919	2.486
338	Phosmet	732-11-6	Daphnia magna	32	55.840	120.590	2.874	-2.459	16.065	1.964	4.753
339	Phosphamidon	13171-21-6	Daphnia magna	37	65.070	7.823	2.743	-2.317	15.585	4.536	4.373
340	Phosphoric acid Divosan X-Tend formulation	7664-38-2	Daphnia magna	8	77.760	7.823	-0.929	0.000	18.994	3.024	-0.030
341	Phostebupirim	96182-53-5	Daphnia magna	44	53.470	126.569	4.222	-2.809	14.760	2.513	6.611
342	Picoxystrobin	117428-22-5	Daphnia magna	42	57.650	12.146	3.840	-3.254	13.508	1.926	4.185
343	Pinoxaden 100 EC formulation	243973-20-8	Daphnia magna	61	62.460	5.969	3.732	-3.853	12.699	1.951	2.291
344	Piperalin	3478-94-2	Daphnia magna	42	29.540	5.969	4.415	-3.347	14.718	1.594	2.242
345	Piperonyl butoxide	51-03-6	Daphnia magna	54	46.150	0.000	3.718	-3.630	12.842	1.518	2.822
346	Pirimicarb	23103-98-2	Daphnia magna	35	58.560	6.093	1.220	-2.645	12.950	2.616	4.564
347	Pirimiphos-methyl	29232-93-7	Daphnia magna	40	56.710	119.502	2.910	-2.459	15.009	2.642	6.163
348	Prallethrin	23031-36-9	Daphnia magna	46	43.370	5.969	3.449	-3.851	12.555	1.914	4.685
349	Profenofos	41198-08-7	Daphnia magna	33	35.530	6.798	5.769	-2.548	19.918	2.534	5.604
350	Prometon	1610-18-0	Daphnia magna	35	71.960	6.010	1.521	-2.500	12.884	2.469	0.943
351	Prometryn	7287-19-6	Daphnia magna	35	62.730	0.000	2.234	-2.500	13.888	2.469	1.113
352	Propachlor	1918-16-7	Daphnia magna	28	20.310	0.000	2.667	-2.991	14.113	2.555	1.487
353	Propargite	2312-35-8	Daphnia magna	51	47.590	148.000	4.517	-3.630	13.511	1.788	3.675
354	Propetamphos	31218-83-4	Daphnia magna	38	56.790	108.242	2.722	-2.404	15.362	4.095	4.931

355	Propiconazole Tilt 3.6 E	60207-90-1	Daphnia magna	39	49.170	0.000	3.653	-3.041	14.777	1.733	2.029
356	Propoxur	114-26-1	Daphnia magna	30	47.560	6.093	2.192	-2.865	12.942	2.419	4.279
357	Propionic acid	79-09-4	Daphnia magna	11	37.300	5.969	0.481	-1.393	13.606	2.540	0.514
358	Prothioconazole (JAU 6476 Technical)	178928-70-6	Daphnia magna	36	53.840	0.000	2.857	-2.928	15.674	1.703	2.458
359	Pymetrozine	123312-89-0	Daphnia magna	27	69.950	6.031	0.817	-2.500	12.884	1.705	0.397
360	Pyraclostrobin	175013-18-0	Daphnia magna	45	65.820	6.093	4.239	-3.346	13.692	1.465	4.393
361	Pyraflufen-ethyl	129630-19-9	Daphnia magna	39	62.580	12.581	4.076	-2.712	15.388	1.988	2.735
362	Pyrethrins	8003-34-7	Daphnia magna	55	69.670	11.939	3.711	-3.874	12.750	1.880	4.507
363	Pyridaben	96489-71-3	Daphnia magna	49	34.890	0.000	5.242	-3.630	14.156	1.778	5.838
364	Pyridalyl	179101-81-6	Daphnia magna	43	40.580	6.176	6.953	-3.015	16.449	1.562	3.135
365	Pyridate	55512-33-9	Daphnia magna	48	52.080	5.301	6.390	-3.529	14.230	1.672	2.545
366	Pyrifluquinazon IV-02 degradate	337458-27-2	Daphnia magna	47	65.540	24.052	4.364	-2.969	14.038	1.779	5.625
367	Pyrimethanil (radiolabeled)	53112-28-0	Daphnia magna	28	37.810	0.000	2.837	-3.126	12.410	1.769	1.817
368	Pyriproxyfen	95737-68-1	Daphnia magna	43	40.580	0.000	4.720	-3.821	12.593	1.260	2.905
369	Quinclorac	84087-01-4	Daphnia magna	20	50.190	5.969	3.240	-2.605	15.801	2.087	0.910
370	Quinoxifen	124495-18-7	Daphnia magna	28	22.120	0.000	5.473	-3.241	15.004	1.602	3.530
371	Quizalofop-ethyl	76578-14-8	Daphnia magna	43	70.540	5.969	4.406	-3.435	13.680	1.421	2.003
372	Quizalofop-P	100646-51-3	Daphnia magna	37	81.540	5.969	3.927	-3.248	13.819	1.375	0.822
373	Resmethrin	10453-86-8	Daphnia magna	51	39.440	5.969	5.152	-4.087	12.490	1.361	6.187
374	Rimsulfuron IN-70942-2 metabolite	122931-48-0	Daphnia magna	45	166.540	6.031	0.193	-2.404	14.797	1.991	0.382
375	Rotenone	83-79-4	Daphnia magna	51	63.220	0.000	3.703	-3.853	12.836	1.347	5.028
376	Ryanodine Ryan 50 powder	15662-33-6	Daphnia magna	70	172.700	5.969	-0.670	-3.664	13.094	1.675	4.050
377	Sedaxane SYN524464 (trans + cis isomers)	874967-67-6	Daphnia magna	43	46.920	0.000	4.124	-3.439	13.009	1.368	1.745
378	Sethoxydim Poast Herbicide formulation	74051-80-2	Daphnia magna	51	58.890	0.000	4.502	-3.446	13.557	2.598	2.100
379	Simazine	122-34-9	Daphnia magna	25	62.730	0.000	1.389	-1.993	14.582	2.330	2.263
380	s-Methoprene	65733-16-6	Daphnia magna	56	35.530	5.969	5.062	-3.851	12.555	3.681	2.936
381	S-Metolachlor	87392-12-9	Daphnia magna	41	29.540	0.000	3.164	-3.354	13.770	2.914	1.038
382	Spinosyn Factor D metabolite	131929-63-0	Daphnia magna	117	111.220	5.969	5.487	-4.495	12.816	1.171	2.285
383	Spiromesifen BSN 2060 SC 240	283594-90-1	Daphnia magna	57	52.600	11.939	5.172	-4.050	12.602	1.854	1.318

formulation											
384	Spiroxamine	118134-30-8	Daphnia magna	56	21.700	0.000	4.066	-3.765	12.486	1.823	2.067
385	Streptomycin	57-92-1	Daphnia magna	77	326.990	0.000	-7.093	-2.794	13.557	1.921	0.205
386	Strychnine	57-24-9	Daphnia magna	47	32.780	0.000	2.093	-3.901	12.490	1.449	1.524
387	Sulfentrazone	122836-35-5	Daphnia magna	33	85.990	12.239	2.416	-2.163	16.396	2.117	0.807
388	Sulfluramid	4151-50-2	Daphnia magna	37	46.170	46.966	4.893	-1.598	16.811	6.838	3.154
389	Sulfotepp	3689-24-5	Daphnia magna	39	46.150	115.316	4.364	-1.924	17.774	4.649	5.110
390	Sulprofos	35400-43-2	Daphnia magna	38	18.460	124.354	5.574	-2.780	16.850	2.404	5.633
391	TCMTB	21564-17-0	Daphnia magna	20	36.680	0.000	3.560	-2.448	16.594	1.700	4.015
392	Tebuconazole	107534-96-3	Daphnia magna	43	50.940	0.000	3.342	-3.347	13.602	1.892	2.029
393	Tebufenozide	112410-23-8	Daphnia magna	54	49.410	0.000	4.452	-3.977	12.471	2.003	1.967
394	Tebufenpyrad	119168-77-3	Daphnia magna	47	46.920	0.000	3.863	-3.540	13.464	1.762	3.919
395	Tebuthiuron	34014-18-1	Daphnia magna	31	58.120	6.031	1.611	-2.344	14.146	2.491	-0.114
396	Tefluthrin	79538-32-2	Daphnia magna	41	26.300	12.146	5.552	-2.994	14.986	1.942	6.777
397	Tembotrione	335104-84-2	Daphnia magna	44	94.580	6.176	2.943	-2.919	15.168	2.144	0.955
398	Temephos Abate 4E formulation	3383-96-8	Daphnia magna	49	55.380	175.952	6.396	-2.818	16.530	1.671	7.627
399	Tepraloxydim (BAS 620 00 H)	149979-41-9	Daphnia magna	47	68.120	0.000	3.739	-3.344	13.811	1.867	1.665
400	Terbacil	5902-51-2	Daphnia magna	27	54.860	5.690	0.772	-2.448	14.540	2.846	0.523
401	Terbufos	13071-79-9	Daphnia magna	37	18.460	108.224	4.889	-2.344	17.818	3.954	5.969
402	Terbutylazine	5915-41-3	Daphnia magna	31	62.730	0.000	2.167	-2.344	14.239	2.442	1.035
403	Terbutryn	886-50-0	Daphnia magna	35	62.730	0.000	2.236	-2.500	13.888	2.500	1.958
404	Tetrachlorvinphos	961-11-5	Daphnia magna	30	63.220	7.823	5.465	-2.092	18.519	2.761	5.321
405	Tetraconazole	112281-77-3	Daphnia magna	34	39.940	12.534	4.243	-2.557	15.698	1.986	2.151
406	Tetrahydro-2(nitromethylene)- 2H-1, 3-thiazine	58842-20-9	Daphnia magna	18	55.170	0.000	0.788	-1.661	15.213	2.131	0.675
407	Tetramethrin	7696-12-0	Daphnia magna	49	63.680	5.969	2.965	-3.630	12.759	1.539	3.867
408	Thiabendazole	148-79-8	Daphnia magna	21	41.570	0.000	2.204	-2.720	13.871	1.615	2.812
409	Thiacloprid	111988-49-9	Daphnia magna	25	52.280	0.000	2.121	-2.500	15.229	1.752	1.050
410	Thiazopyr	117718-60-2	Daphnia magna	43	51.550	12.146	4.517	-2.893	14.586	2.487	1.813
411	Thidiazuron	51707-55-2	Daphnia magna	23	66.910	6.031	2.182	-2.344	14.146	1.637	1.587
412	Thiencarbazone methyl M15 degradate	317815-83-1	Daphnia magna	39	138.590	23.701	-0.306	-2.229	15.051	2.087	1.922
413	Thiobencarb	28249-77-6	Daphnia magna	32	20.310	0.000	4.035	-3.000	15.104	2.181	3.406

414	Thiodicarb	59669-26-0	Daphnia magna	39	75.960	12.190	2.601	-2.092	16.016	2.815	4.118
415	Thiophanate-methyl	23564-05-8	Daphnia magna	36	100.720	12.186	1.792	-2.432	14.922	2.448	1.810
416	Tolclofos-methyl	57018-04-9	Daphnia magna	28	27.690	110.801	4.581	-2.250	18.128	2.645	0.798
417	Tolfenpyrad	129558-76-5	Daphnia magna	49	56.150	0.000	4.667	-3.698	13.396	1.344	5.584
418	Tolyfluanid	731-27-1	Daphnia magna	32	40.620	14.128	3.314	-2.236	17.587	2.862	3.262
419	Tolyfluanid DMST metabolite	66840-71-9	Daphnia magna	28	49.410	10.209	1.213	-2.448	14.298	2.372	0.838
420	Toxaphene (Cancelled in U.S.)	8001-35-2	Daphnia magna	26	0.000	0.000	6.073	-2.317	22.430	2.903	4.615
421	Tralkoxydim JF9517 formulation	87820-88-0	Daphnia magna	51	58.890	0.000	4.673	-3.821	12.593	2.036	2.223
422	Tralomethrin	66841-25-6	Daphnia magna	49	59.320	5.969	7.461	-3.598	21.529	1.549	7.232
423	Triadimefon	43121-43-3	Daphnia magna	36	57.010	0.000	3.124	-3.025	13.881	1.984	2.230
424	Triadimenol	55219-65-3	Daphnia magna	38	60.170	0.000	2.916	-3.025	13.881	1.984	2.073
425	Triallate	2303-17-5	Daphnia magna	32	20.310	0.000	4.844	-2.500	18.034	4.161	3.525
426	Triazamate	112143-82-5	Daphnia magna	43	77.320	12.000	1.760	-2.719	13.916	2.673	4.351
427	Tribufos	78-48-8	Daphnia magna	44	17.070	0.000	6.694	-2.885	16.900	3.946	4.665
428	Tributyltin fluoride(TBTF)	1983-10-4	Daphnia magna	41	0.000	94.422	5.302	-3.263	20.131	3.890	6.096
429	Tributyltin oxide	56-35-9	Daphnia magna	81	9.230	184.206	9.695	-4.227	20.062	5.663	5.553
430	Trichloromelamine	7673-09-8	Daphnia magna	15	74.760	0.000	1.569	-0.896	18.870	2.405	2.282
431	Trichloro-s-triazinetriene	87-90-1	Daphnia magna	12	66.000	17.069	-0.823	-0.896	19.367	2.760	3.136
432	Triclopyr acid	55335-06-3	Daphnia magna	18	59.420	5.969	2.505	-1.904	18.031	2.368	0.286
433	Triclopyr butoxyethyl ester (Garlon 4)	64700-56-7	Daphnia magna	37	57.650	5.969	3.781	-2.719	16.215	2.078	3.008
434	Triclosan	3380-34-5	Daphnia magna	24	29.460	0.000	5.145	-2.885	16.617	1.837	2.871
435	Tricosene	27519-02-4	Daphnia magna	69	0.000	0.000	8.994	-4.524	12.011	2.922	3.085
436	Tridecen-1-yl acetate (Z and E acetates)	65954-19-0	Daphnia magna	45	26.300	5.969	4.637	-3.607	12.480	2.893	2.649
437	Tridiphane (DOWCO 356)	58138-08-2	Daphnia magna	23	12.530	0.000	4.979	-2.500	19.586	2.006	3.108
438	Trifloxystrobin	141517-21-7	Daphnia magna	48	69.480	12.146	4.170	-3.350	13.422	1.849	4.208
439	Trifluralin	1582-09-8	Daphnia magna	39	89.520	6.176	4.148	-2.557	13.876	3.148	3.126
440	Triforine	26644-46-2	Daphnia magna	36	64.680	0.000	1.489	-2.027	19.130	2.678	1.191
441	Trimethacarb	2686-99-9	Daphnia magna	29	38.330	6.093	2.330	-2.991	12.723	2.485	4.031
442	Tris(hydroxymethyl)nitromethane	126-11-4	Daphnia magna	19	103.830	0.000	-2.021	-1.329	14.205	4.154	0.276
443	Triticonazole	131983-72-7	Daphnia magna	42	50.940	0.000	3.566	-3.446	13.530	1.656	1.621
444	Vinclozolin	50471-44-8	Daphnia magna	27	46.610	6.093	3.421	-2.780	15.391	2.125	1.894

445	Warfarin	81-81-2	Daphnia magna	39	67.510	5.626	3.610	-3.737	12.705	1.778	0.644
446	Acrolein	107-02-8	Americamysis bahia	8	17.070	0.000	0.371	-1.500	13.008	1.975	2.050
447	Bifenox	42576-02-3	Americamysis bahia	31	78.670	5.969	4.481	-2.838	15.139	1.928	3.911
448	Butafenacil	134605-64-4	Americamysis bahia	50	96.600	23.805	2.873	-3.125	14.271	2.090	3.530
449	Carfentrazone-ethyl	128639-02-1	Americamysis bahia	40	66.120	18.208	3.243	-2.712	15.311	2.052	2.551
450	Cimecticarb	95266-40-3	Americamysis bahia	34	80.670	5.969	1.320	-3.012	13.119	1.937	1.589
451	Clothianidin	210880-92-5	Americamysis bahia	23	92.450	0.000	0.653	-1.563	16.108	2.160	3.690
452	Cyclanilide	113136-77-9	Americamysis bahia	26	69.890	5.969	3.446	-2.645	15.590	1.885	1.739
453	Dicofol	115-32-2	Americamysis bahia	29	20.230	0.000	5.600	-3.025	18.071	2.172	3.791
454	Dieldrin (Cancelled in U.S.)	60-57-1	Americamysis bahia	27	12.530	0.000	4.481	-2.683	19.624	1.758	5.013
455	Dimethoate	60-51-5	Americamysis bahia	25	51.050	81.815	2.206	-1.494	18.097	3.720	1.184
456	Dimethomorph	110488-70-5	Americamysis bahia	49	48.000	0.000	3.648	-3.698	13.544	1.669	1.070
457	Dinotefuran	165252-70-0	Americamysis bahia	28	88.790	0.000	-0.620	-1.904	13.436	2.123	2.408
458	EPN (Cancelled in U.S.)	2104-64-5	Americamysis bahia	36	61.600	128.121	4.028	-2.928	14.724	1.899	4.978
459	Flufenacet	142459-58-3	Americamysis bahia	37	55.320	6.176	3.516	-2.675	14.593	1.820	2.126
460	Flufenpyr-ethyl	188489-07-8	Americamysis bahia	40	70.420	12.146	3.294	-2.818	14.653	2.014	2.289
461	Flumetralin	62924-70-3	Americamysis bahia	40	89.520	6.176	5.341	-2.747	14.630	2.300	3.652
462	Flumiclorac	87546-18-7	Americamysis bahia	37	83.910	5.969	2.686	-3.057	14.193	1.715	2.800
463	Fluthiacet methyl	117337-19-6	Americamysis	40	65.590	10.842	2.795	-2.786	15.551	1.568	3.159

			bahia								
464	Flutolanil	66332-96-5	Americamysis bahia	39	41.820	6.176	5.129	-3.344	13.356	1.901	3.396
465	Halosulfuron methyl	100784-20-1	Americamysis bahia	43	163.630	12.000	0.178	-2.232	14.989	2.014	0.601
466	Heptachlor (Cancelled in U.S.)	76-44-8	Americamysis bahia	22	0.000	0.000	5.094	-2.404	21.664	2.137	5.041
467	Isoxaflutole	141112-29-0	Americamysis bahia	36	77.240	6.176	3.205	-2.866	14.468	1.749	4.305
468	Maneb 80WP	12427-38-2	Americamysis bahia	17	24.060	89.875	1.128	-1.258	23.569	2.237	4.905
469	Mefenoxam A13947A formulation	70630-17-0	Americamysis bahia	41	55.840	5.969	1.844	-3.241	12.908	2.950	1.591
470	Metronidazole	443-48-1	Americamysis bahia	21	81.190	5.818	0.092	-1.792	13.507	2.510	-0.027
471	Mevinphos	7786-34-7	Americamysis bahia	27	71.060	13.792	1.481	-1.904	15.075	3.964	5.237
472	Molinate	2212-67-1	Americamysis bahia	26	20.310	0.000	2.345	-2.516	14.378	2.205	2.358
473	Norflurazon	27314-13-2	Americamysis bahia	29	46.920	6.176	2.946	-2.593	14.730	2.006	1.740
474	Penflufen	494793-67-8	Americamysis bahia	33	58.200	12.207	3.946	-2.866	13.965	1.758	2.139
475	Primisulfuron-methyl	86209-51-0	Americamysis bahia	43	146.490	30.342	-0.308	-2.397	14.718	1.747	1.466
476	Prodiamine	29091-21-2	Americamysis bahia	41	115.540	11.864	3.730	-2.484	13.882	3.286	2.222
477	Propanil	709-98-8	Americamysis bahia	22	29.100	0.000	3.342	-2.562	16.078	2.287	2.748
478	Propyzamide	23950-58-5	Americamysis bahia	27	32.590	0.000	3.710	-3.000	15.315	2.496	1.600
479	Pyrasulfotole	365400-11-9	Americamysis bahia	37	89.260	6.176	2.087	-2.675	14.551	2.214	2.518
480	Saflufenacil	372137-35-4	Americamysis bahia	49	110.480	22.075	1.662	-2.656	15.116	2.199	1.770
481	Spirotetramat	203313-25-1	Americamysis	54	73.860	6.155	3.645	-3.698	12.823	1.837	1.832

			bahia								
482	Sulfoxaflor	946578-00-3	Americamysis bahia	28	70.680	6.176	2.942	-2.317	14.844	2.524	2.617
483	Thiamethoxam	153719-23-4	Americamysis bahia	28	84.100	0.000	1.023	-1.853	15.647	1.904	1.626
484	Thiram	137-26-8	Americamysis bahia	26	6.480	86.908	2.245	-1.792	19.029	1.848	4.855
485	Topramezone	210631-68-8	Americamysis bahia	42	110.850	0.000	1.193	-2.972	13.850	1.783	2.129
486	Triethylene glycol	112-27-6	Americamysis bahia	24	58.920	0.000	-0.996	-1.993	13.606	2.648	-1.865
487	Triflumizole	68694-11-1	Americamysis bahia	38	39.410	6.176	4.560	-2.950	14.375	1.997	2.761
488	Zoxamide	156052-68-5	Americamysis bahia	36	46.170	0.000	4.008	-3.025	16.026	2.678	3.652
489	Allethrin	584-79-2	Gammarus fasciatus	48	43.370	5.969	4.002	-3.851	12.555	1.914	4.439
490	Antimycin A	1397-94-0	Gammarus fasciatus	79	157.330	17.908	3.480	-3.795	13.034	2.209	7.836
491	Benzyl benzoate	120-51-4	Gammarus fasciatus	28	26.300	5.969	3.044	-3.500	12.509	1.633	1.646
492	Cacodylic acid	75-60-5	Gammarus fasciatus	12	37.300	33.089	0.111	-0.929	26.188	3.024	0.010
493	Crotoxyphos	7700-17-6	Gammarus fasciatus	40	71.060	13.792	3.612	-2.928	14.053	2.325	4.456
494	Cruformate (Ruelene 8R)	299-86-5	Gammarus fasciatus	37	47.560	7.746	3.990	-2.780	15.142	2.579	1.897
495	Demeton	8065-48-3	Gammarus fasciatus	33	35.530	6.798	3.654	-2.176	17.085	3.709	3.731
496	Dichloro diphenyl dichlorethane (TDE)	72-54-8	Gammarus fasciatus	28	0.000	0.000	5.929	-3.243	17.220	1.949	5.727
497	EPN (Cancelled in U.S.)	2104-64-5	Gammarus fasciatus	36	61.600	128.121	4.028	-2.928	14.724	1.899	4.677
498	Heptachlor (Cancelled in U.S.)	76-44-8	Gammarus fasciatus	22	0.000	0.000	5.094	-2.404	21.664	2.137	4.110
499	Methoxychlor	72-43-5	Gammarus	36	18.460	0.000	5.206	-3.347	15.740	1.991	5.260

500	Mevinphos	7786-34-7	fasciatus Gammarus	27	71.060	13.792	1.481	-1.904	15.075	3.964	4.903
501	Monocrotophos (Cancelled in U.S.)	6923-22-4	fasciatus Gammarus	28	77.350	7.823	1.894	-1.904	14.932	3.964	2.934
502	Picloram	1918-02-1	fasciatus Gammarus	16	76.210	5.969	2.322	-1.708	18.341	2.701	0.951
503	Tetraethyl pyrophosphate (TEPP)	107-49-3	fasciatus	37	80.290	15.645	3.365	-1.924	15.884	4.649	3.140
504	Dieldrin (Cancelled in U.S.)	60-57-1	Penaeus duorarum	27	12.530	0.000	4.481	-2.683	19.624	1.758	6.104
505	Dinoseb acid (Cancelled in U.S.)	88-85-7	Penaeus duorarum	29	106.510	5.687	2.722	-2.404	13.419	2.818	2.088
506	EPN (Cancelled in U.S.)	2104-64-5	Penaeus duorarum	36	61.600	128.121	4.028	-2.928	14.724	1.899	6.047
507	Glyphosine (Polaris formula)	2439-99-8	Penaeus duorarum	26	155.600	21.161	-1.357	-1.042	16.799	4.322	0.015
508	Heptachlor (Cancelled in U.S.)	76-44-8	Penaeus duorarum	22	0.000	0.000	5.094	-2.404	21.664	2.137	7.095
509	MCPA acid	94-74-6	Penaeus duorarum	22	46.530	5.969	2.112	-2.562	14.735	2.254	-0.071
510	Phorate	298-02-2	Penaeus duorarum	31	18.460	95.383	4.111	-1.993	18.712	3.764	6.374
511	Trichlorfon	52-68-6	Penaeus duorarum	20	55.760	7.596	2.161	-1.195	20.781	4.527	5.854

Table S2: Data set used in ISC QSAAR modeling

S.No.	Chemical name	CAS No.	Taxonomic name	LogP	pEC ₅₀ (mM) (Daphnia magna)	pLC ₅₀ (mM)
1	(S)-Dimethenamid	163515-14-8	Lepomis macrochirus	2.972	1.361	1.441
2	1,2-Benzisothiazolin-3-one	2634-33-5	Lepomis macrochirus	1.108	2.138	2.447
3	1,2-Benzisothiazolin-3-one, 2-butyl	4299-07-4	Lepomis macrochirus	2.863	3.330	2.584
4	1,3 Dichloropropene (Telone soil fumigant)	542-75-6	Lepomis macrochirus	1.978	3.091	1.477
5	1,3,5-Triethylhexahydro-s-triazine, VancideTH	7779-27-3	Lepomis macrochirus	0.838	1.049	0.745
6	1,4-Bis(bromoacetoxy)-2-butene (BBAB)	20679-58-7	Lepomis macrochirus	1.419	3.372	3.763

7	2,4-D Acid	94-75-7	Lepomis macrochirus	2.457	0.947	0.089
8	2,4-D Butoxyethanol Ester	1929-73-3	Lepomis macrochirus	3.732	2.276	2.721
9	2,4-D Isopropyl Ester	94-11-1	Lepomis macrochirus	3.324	2.005	2.929
10	2,4-D Propylene Glycol B.E. Ester	1320-18-9	Lepomis macrochirus	4.121	2.446	2.777
11	2,4-DB Acid	94-82-6	Lepomis macrochirus	3.237	0.993	1.521
12	2,4-DP 2-Butoxyethyl Ester Weedone formula	53404-31-2	Lepomis macrochirus	4.121	4.729	2.605
13	2-Benzyl-4-chlorophenol (Nipacide BCP)	120-32-1	Lepomis macrochirus	3.636	2.569	2.821
14	2-Bromo-4'-hydroxyacetophenone (BHAP)	2491-38-5	Lepomis macrochirus	1.97	1.500	1.961
15	2-EEEBC (Debacarb)	62732-91-6	Lepomis macrochirus	1.683	-0.964	-0.378
16	2-Hydroxyacetophenone 2-Hydroxyethyl octyl sulfide	118-93-4	Lepomis macrochirus	0.862	0.456	0.073
17	MGK 874 repellent 2-Hydroxypropyl	3547-33-9	Lepomis macrochirus	3.072	2.711	1.832
18	methanethiosulfonate(HPMTS)	30388-01-3	Lepomis macrochirus	0.06	1.152	0.649
19	3,5 Dimethyl-1- (hydroxymethyl)pyrazole	85264-33-1	Lepomis macrochirus	0.45	0.600	0.209
20	3-Iodo-2-propynyl butyl carbamate (IPBC)	55406-53-6	Lepomis macrochirus	1.909	3.245	3.095
21	4,4-Dimethyloxazolidine	51200-87-4	Lepomis macrochirus	0.342	0.352	0.234
22	4,5-Dichloro-2-n-octyl-3(2H)- isothiazolone	64359-81-5	Lepomis macrochirus	3.709	4.733	4.304
23	4-Chloro-3,5-xyleneol (Ottasept))	88-04-0	Lepomis macrochirus	2.662	1.763	1.991
24	Acetochlor WF2061 formulation	34256-82-1	Lepomis macrochirus	3.123	1.574	2.317
25	Acibenzolar-s-methyl	135158-54-2	Lepomis macrochirus	2.195	1.860	2.119
26	Aldicarb	116-06-3	Lepomis macrochirus	1.47	2.666	3.478
27	Aldoxycarb	1646-88-4	Lepomis macrochirus	0.151	2.900	0.623
28	Ametryn	834-12-8	Lepomis macrochirus	1.846	0.909	1.788
29	Amitraz	33089-61-1	Lepomis macrochirus	4.872	1.939	2.936
30	Anilazine	101-05-3	Lepomis macrochirus	3.575	2.463	2.935
31	Aspon (Ortho Sod-Cancelled in U.S.)	3244-90-4	Lepomis macrochirus	5.924	5.758	3.578

32	Atrazine	1912-24-9	Lepomis macrochirus	1.777	1.495	1.508
33	Azadirachtin	108168-76-9	Lepomis macrochirus	0.942	1.889	1.290
34	Azinphos-methyl	86-50-0	Lepomis macrochirus	2.382	5.448	4.889
35	Azoxystrobin	131860-33-8	Lepomis macrochirus	4.093	3.192	2.564
36	BCDM Hydantoin, 1-bromo-3-chloro-5,5-dimethyl	16079-88-2	Lepomis macrochirus	1.493	2.650	2.827
37	Bendiocarb	22781-23-3	Lepomis macrochirus	1.912	3.883	2.677
38	Benfluralin Balan EC formulation	1861-40-1	Lepomis macrochirus	4.148	2.186	3.712
39	Benomyl 50WP formulation	17804-35-2	Lepomis macrochirus	2.572	3.329	3.040
40	Bensulide	741-58-2	Lepomis macrochirus	4.423	2.836	2.691
41	Benzyl bromoacetate	5437-45-6	Lepomis macrochirus	2.125	2.998	3.307
42	Bethoxazin BTCN metabolite (Canceled in U.S.)	163269-30-5	Lepomis macrochirus	2.94	2.196	2.157
43	Bifenazate	149877-41-8	Lepomis macrochirus	3.824	2.779	2.714
44	Bifenthrin	82657-04-3	Lepomis macrochirus	6.662	5.422	6.090
45	Bioresmethrin	28434-01-7	Lepomis macrochirus	5.152	5.626	5.626
46	Bis (3-aminopropyl)dodecylamine)					
46	Lonzabac 12	2372-82-9	Lepomis macrochirus	3.907	3.613	2.823
47	Bis (trichloromethyl) sulfone	3064-70-8	Lepomis macrochirus	3.057	3.240	3.715
48	Bitertanol	55179-31-2	Lepomis macrochirus	3.93	1.856	2.206
49	Brodifacoum	56073-10-0	Lepomis macrochirus	7.79	2.728	3.640
50	Bromacil	314-40-9	Lepomis macrochirus	1.097	0.334	0.313
51	Bromadiolone	28772-56-7	Lepomis macrochirus	7.184	3.342	2.245
52	Bromonitrostyrene	7166-19-0	Lepomis macrochirus	2.657	3.978	4.128
53	Bromoxynil AXF 1240 formulation	1689-84-5	Lepomis macrochirus	2.789	0.573	1.081
54	Bromoxynil butyrate	3861-41-4	Lepomis macrochirus	3.789	3.239	3.888
55	Bromoxynil heptanoate	56634-95-8	Lepomis macrochirus	4.959	4.099	4.128
56	Bromoxynil octanoate	1689-99-2	Lepomis macrochirus	5.349	3.549	3.835
57	Bromuconazole (EXP 10064)	116255-48-2	Lepomis macrochirus	3.664	3.647	1.953
58	Bronopol	52-51-7	Lepomis macrochirus	-0.661	2.097	1.253

59	Butralin	33629-47-9	Lepomis macrochirus	4.011	3.391	2.470
60	Butylate	2008-41-5	Lepomis macrochirus	3.372	1.233	2.986
61	Cadusafos	95465-99-9	Lepomis macrochirus	5.194	5.172	3.199
62	Carbofuran	1563-66-2	Lepomis macrochirus	2.118	3.882	2.532
63	Carboxin	5234-68-4	Lepomis macrochirus	2.62	0.445	2.292
64	Chlorethoxyfos	54593-83-8	Lepomis macrochirus	4.619	5.914	5.165
65	Chlorfenapyr	122453-73-0	Lepomis macrochirus	5.455	4.718	4.546
66	Chlorflurenol methyl ester	37339-61-0	Lepomis macrochirus	2.729	1.564	2.108
67	Chloroneb	2675-77-6	Lepomis macrochirus	3.011	1.524	1.626
68	Chlorophacinone	3691-35-8	Lepomis macrochirus	4.736	2.944	2.734
69	Chloropicrin	76-06-2	Lepomis macrochirus	1.591	3.137	3.571
70	Chlorothalonil(Degradate)	1897-45-6	Lepomis macrochirus	4.044	1.010	1.221
71	Chlorpropham	101-21-3	Lepomis macrochirus	3.297	1.762	1.497
72	Chlorpyrifos	2921-88-2	Lepomis macrochirus	5.101	6.545	5.431
73	Chromic acid	7738-94-5	Lepomis macrochirus	-1.354	2.191	0.428
74	Cinnamaldehyde	104-55-2	Lepomis macrochirus	1.899	1.273	1.645
75	Clomazone	81777-89-1	Lepomis macrochirus	2.64	1.664	0.848
76	Cyanamide (Alzodef)	420-04-2	Lepomis macrochirus	-0.574	0.798	-0.321
77	Cyanazine	21725-46-2	Lepomis macrochirus	1.671	0.758	1.029
78	Cyfluthrin (Tempo 2EC Formulation)	68359-37-5	Lepomis macrochirus	6.317	7.240	5.698
79	Cyhalothrin	68085-85-8	Lepomis macrochirus	6.544	6.073	5.990
80	Cyhexatin	13121-70-5	Lepomis macrochirus	5.927	6.355	5.017
81	Cymoxanil	57966-95-7	Lepomis macrochirus	-0.642	2.394	0.835
82	Cypermethrin Beta	52315-07-8	Lepomis macrochirus	6.178	5.996	5.540
83	Cyproconazole	94361-06-5	Lepomis macrochirus	2.865	1.050	1.143
84	Cyprodinil	121552-61-2	Lepomis macrochirus	3.406	3.848	2.014
85	Daminozide	1596-84-5	Lepomis macrochirus	-0.556	0.211	-0.422
86	Dazomet	533-74-4	Lepomis macrochirus	0.797	2.692	2.733
87	DBDMH Glybrom formulation	77-48-5	Lepomis macrochirus	1.649	2.532	3.025
88	DBNPA	10222-01-2	Lepomis macrochirus	0.481	2.449	2.270

89	DCDMH (Dantochlor Formulation)	118-52-5	Lepomis macrochirus	1.337	2.622	1.927
90	DDT (Cancelled in U.S.)	50-29-3	Lepomis macrochirus	6.496	4.878	5.345
91	Decanol (Alfol 810 alcohol)	112-30-1	Lepomis macrochirus	3.119	1.386	1.496
92	Deltamethrin	52918-63-5	Lepomis macrochirus	6.49	6.662	6.147
93	Desmedipham	13684-56-5	Lepomis macrochirus	3.866	2.203	1.699
94	Diazinon	333-41-5	Lepomis macrochirus	3.968	5.766	3.524
95	Dibromodicyanobutane	35691-65-7	Lepomis macrochirus	2.546	2.082	1.812
96	Dicamba	1918-00-9	Lepomis macrochirus	2.7	0.300	0.213
97	Dichlobenil	1194-65-6	Lepomis macrochirus	2.865	1.443	1.408
98	Dichlorprop (2,4-DP) Weedone formulation	120-36-5	Lepomis macrochirus	2.845	4.647	2.452
99	Dichlorvos in Muscalure Z-9 formulation	62-73-7	Lepomis macrochirus	2.68	2.311	2.425
100	Diclofop-methyl	51338-27-3	Lepomis macrochirus	4.726	3.171	3.357
101	Dicloran (DCNA)	99-30-9	Lepomis macrochirus	2.484	2.000	2.283
102	Dienochlor	2227-17-0	Lepomis macrochirus	7.726	2.597	2.898
103	Difenoconazole	119446-68-3	Lepomis macrochirus	4.666	2.722	2.530
104	Difethialone	104653-34-1	Lepomis macrochirus	8.259	5.089	3.857
105	Diiodomethyl p-tolyl sulfone (Amical 48)	20018-09-1	Lepomis macrochirus	2.922	3.774	2.750
106	Dimethenamid	87674-68-8	Lepomis macrochirus	2.972	1.236	1.634
107	Dimethepin (Harvade 25F formulation)	55290-64-7	Lepomis macrochirus	0.081	1.503	1.003
108	Dinitramine	29091-05-2	Lepomis macrochirus	2.95	2.394	1.752
109	Dinocap	39300-45-3	Lepomis macrochirus	5.058	4.938	4.261
110	Diphacinone	82-66-6	Lepomis macrochirus	4.083	2.277	1.651
111	Diphenamid	957-51-7	Lepomis macrochirus	2.907	0.616	0.566
112	Dipropyl isocinchomeronate MGK 326 repellent	136-45-8	Lepomis macrochirus	2.215	1.145	2.757
113	Disulfoton	298-04-4	Lepomis macrochirus	4.421	4.324	3.847
114	Dithiopyr Dimension formulation	97886-45-8	Lepomis macrochirus	5.243	1.888	2.931
115	Diuron Karmex DF Formulation	330-54-1	Lepomis macrochirus	3.087	1.443	1.920

116	D-Phenothrin (Sumithrin)	26002-80-2	Lepomis macrochirus	5.761	4.901	4.346
117	DTEA	36362-09-1	Lepomis macrochirus	3.819	3.781	2.492
118	d-trans-Allethrin	584-79-2	Lepomis macrochirus	4.002	4.531	4.128
119	Endothall	145-73-3	Lepomis macrochirus	-0.051	0.758	1.636
120	Esfenvalerate Ethalfluralin Sonalan EC	66230-04-4	Lepomis macrochirus	6.68	6.447	6.261
121	formulation	55283-68-6	Lepomis macrochirus	3.924	4.265	4.018
122	Ethephon	16672-87-0	Lepomis macrochirus	0.403	0.659	0.099
123	Ethofenprox	80844-07-1	Lepomis macrochirus	6.372	5.820	5.203
124	Ethofumesate	26225-79-6	Lepomis macrochirus	2.058	0.651	2.059
125	Ethoprop Ethyl N,N-dipropylthiocarbamate	13194-48-4	Lepomis macrochirus	4.417	3.753	2.907
126	(EPTC)	759-94-4	Lepomis macrochirus	2.982	1.128	1.131
127	Famoxadone Fenamidone(RPA413255 s-	131807-57-3	Lepomis macrochirus	4.7	4.501	4.459
128	enantiomer) Fenamiphos Nemacur 3	161326-34-7	Lepomis macrochirus	3.49	1.507	2.624
129	formulation	22224-92-6	Lepomis macrochirus	4.238	5.368	4.834
130	Fenarimol	60168-88-9	Lepomis macrochirus	4.068	1.688	2.566
131	Fenazaquin	120928-09-8	Lepomis macrochirus	4.549	4.738	3.954
132	Fenbuconazole	114369-43-6	Lepomis macrochirus	4.026	2.166	2.695
133	Fenbutatin oxide	13356-08-6	Lepomis macrochirus	16.761	4.531	5.341
134	Fenhexamid	126833-17-8	Lepomis macrochirus	4.608	0.459	1.946
135	Fenoxaprop-ethyl	66441-23-4	Lepomis macrochirus	4.604	2.056	3.067
136	Fenoxycarb	72490-01-8	Lepomis macrochirus	3.604	2.877	2.610
137	Fenpropathrin	39515-41-8	Lepomis macrochirus	5.269	5.819	5.201
138	Fenpyroximate FujiMite 5EC	134098-61-6	Lepomis macrochirus	5.027	5.421	5.324
139	Fenvalerate	51630-58-1	Lepomis macrochirus	6.68	6.924	6.000
140	Fipronil MB 46136 metabolite	120068-37-3	Lepomis macrochirus	4.877	4.178	4.340
141	Fluazifop-butyl (PP009)	69806-50-4	Lepomis macrochirus	5.003	1.804	2.859
142	Fluazinam	79622-59-6	Lepomis macrochirus	5.986	3.412	3.946
143	Fludioxonil(Maxim 4FS)	131341-86-1	Lepomis macrochirus	2.393	2.441	2.531

144	Fluometuron	2164-17-2	Lepomis macrochirus	2.799	1.370	1.236
145	Fluoxastrobin	361377-29-9	Lepomis macrochirus	4.565	2.980	2.675
146	Fluridone	59756-60-4	Lepomis macrochirus	4.738	2.040	1.705
147	Flurprimidol	56425-91-3	Lepomis macrochirus	3.267	1.482	1.312
148	Flutriafol 125 g/L SC formulation	76674-21-0	Lepomis macrochirus	2.492	1.631	0.960
149	Fluvalinate	69409-94-5	Lepomis macrochirus	7.396	6.099	5.916
150	Fluxapyroxad	907204-31-3	Lepomis macrochirus	4.694	1.750	2.521
151	Folpet	133-07-3	Lepomis macrochirus	3.259	2.735	3.800
152	Fonofos	944-22-9	Lepomis macrochirus	4.528	5.082	4.559
153	Forchlorfenuron	68157-60-8	Lepomis macrochirus	3.379	1.670	1.449
154	Fosthiazate	98886-44-3	Lepomis macrochirus	3.832	3.037	1.643
155	Furfural	98-01-1	Lepomis macrochirus	1.092	0.673	1.219
156	Gamma cyhalothrin	76703-62-3	Lepomis macrochirus	6.544	7.000	7.197
157	Glutaraldehyde	111-30-8	Lepomis macrochirus	0.554	2.125	0.914
158	Glyphosate N-(phosphonomethyl) glycine	1071-83-6	Lepomis macrochirus	-1.204	0.101	0.575
159	Grotan	4719-04-4	Lepomis macrochirus	-2.245	0.924	0.750
160	Hexaconazole JF 9445 formulation - test 1	79983-71-4	Lepomis macrochirus	3.663	2.218	1.790
161	Hexazinone	51235-04-2	Lepomis macrochirus	0.513	0.473	0.025
162	Hexythiazox PT-1-9	78587-05-0	Lepomis macrochirus	4.981	1.652	2.823
163	Hydramethylnon	67485-29-4	Lepomis macrochirus	6.382	2.637	2.464
164	Imazalil	35554-44-0	Lepomis macrochirus	4.134	1.973	1.872
165	Imazamethabenz	81405-85-8	Lepomis macrochirus	2.073	0.117	-0.163
166	Imazaquin	81335-37-7	Lepomis macrochirus	2.224	0.046	-0.130
167	Imiprothrin (Pralle)	72963-72-5	Lepomis macrochirus	1.623	3.795	3.658
168	Iprodione	36734-19-7	Lepomis macrochirus	2.88	3.139	1.951
169	Irgarol	28159-98-0	Lepomis macrochirus	2.378	1.679	1.989
170	Isazophos methyl Triumph 4E formulation	42509-83-1	Lepomis macrochirus	2.791	5.113	4.873
171	Kepone (Cancelled in U.S.)	143-50-0	Lepomis macrochirus	4.823	3.276	3.833
172	Kresoxim methyl	143390-89-0	Lepomis macrochirus	2.611	2.975	2.798

173	Lactofen	77501-63-4	Lepomis macrochirus	5.168	2.363	2.342
174	Lambda-Cyhalothrin	91465-08-6	Lepomis macrochirus	6.544	7.051	6.628
175	Linuron	330-55-2	Lepomis macrochirus	3.019	3.317	1.433
176	L-Lactic acid	79-33-4	Lepomis macrochirus	-0.548	-0.920	-0.159
177	Malathion	121-75-5	Lepomis macrochirus	2.505	5.519	4.218
178	Maleic hydrazide	123-33-1	Lepomis macrochirus	-1.901	0.018	-1.157
179	MCPA 2-ethylhexyl ester	29450-45-1	Lepomis macrochirus	4.787	3.048	1.990
180	Metalaxyl Ridomil 2E-G	57837-19-1	Lepomis macrochirus	1.844	1.349	1.015
181	Methiocarb	2032-65-7	Lepomis macrochirus	2.744	4.074	3.031
182	Methomyl	16752-77-5	Lepomis macrochirus	1.039	4.266	2.642
183	Methoprene	40596-69-8	Lepomis macrochirus	5.062	2.543	2.310
184	Methyl anthralinate	134-20-3	Lepomis macrochirus	1.055	0.919	1.219
185	Methyl chloroform	71-55-6	Lepomis macrochirus	2.377	1.076	0.362
186	Methyl isothiocyanate	556-61-6	Lepomis macrochirus	0.719	2.983	2.785
187	Methyl nonyl ketone	112-12-9	Lepomis macrochirus	3.716	2.499	1.909
188	Methylene bis(thiocyanate) Slime- trol RX32	6317-18-6	Lepomis macrochirus	1.372	1.569	1.862
189	Metolachlor CGA-51502	51218-45-2	Lepomis macrochirus	3.164	1.265	1.453
190	Metribuzin	21087-64-9	Lepomis macrochirus	0.372	1.710	0.450
191	Mexacarbate (Zectran)	315-18-4	Lepomis macrochirus	2.088	3.734	1.713
192	MGK-264	113-48-4	Lepomis macrochirus	3.006	2.078	2.060
193	Myclobutanil	88671-89-0	Lepomis macrochirus	3.583	1.419	2.080
194	Naphthalene	91-20-3	Lepomis macrochirus	2.84	1.904	1.603
195	Naphthaleneacetate acid ethyl ester	2122-70-5	Lepomis macrochirus	2.945	0.954	1.903
196	Naphthaleneacetic acid	86-87-3	Lepomis macrochirus	2.467	0.015	0.895
197	Napropamide	15299-99-7	Lepomis macrochirus	3.476	1.278	1.354
198	Niclosamide	1420-04-8	Lepomis macrochirus	3.86	3.214	3.333
199	Nitrapyrin	1929-82-4	Lepomis macrochirus	3.562	2.021	1.832
200	N-Methyl-2-pyrrolidine N-methylneodecanamide	120-94-5	Lepomis macrochirus	0.712	-1.769	-0.990
201	(MNDA)	105726-67-8	Lepomis macrochirus	2.729	0.154	0.314

202	OBPA	58-36-6	Lepomis macrochirus	2.826	5.020	4.798
203	Octhilinone	26530-20-1	Lepomis macrochirus	2.576	3.300	3.125
204	Ortho-phenyl phenol	90-43-7	Lepomis macrochirus	3.059	1.831	1.761
205	Oryzalin	19044-88-3	Lepomis macrochirus	1.777	2.363	2.080
206	Oxadiazon	19666-30-9	Lepomis macrochirus	4.217	2.814	2.594
207	Oxamyl	23135-22-0	Lepomis macrochirus	0.107	2.669	1.593
208	Oxazolidine E	7747-35-5	Lepomis macrochirus	0.413	0.533	0.042
209	Oxycarboxin	5259-88-1	Lepomis macrochirus	1.302	0.588	0.978
210	Oxydemeton-methyl	301-12-2	Lepomis macrochirus	2.487	3.187	2.305
211	Oxyfluorfen	42874-03-3	Lepomis macrochirus	5.458	3.655	3.257
212	Oxythioquinox	2439-01-2	Lepomis macrochirus	2.575	3.291	3.846
213	Paclbutrazol	76738-62-0	Lepomis macrochirus	3.122	0.947	1.095
214	Paranitrophenol	100-02-7	Lepomis macrochirus	1.3	1.365	1.324
215	Parathion 8E Formulation	56-38-2	Lepomis macrochirus	3.654	4.987	4.209
216	Pebulate	1114-71-2	Lepomis macrochirus	3.372	1.474	1.411
217	Pendimethalin	40487-42-1	Lepomis macrochirus	3.72	3.002	3.150
218	Pentachloronitrobenzene (PCNB)	82-68-8	Lepomis macrochirus	4.862	2.584	3.470
219	Pentachlorophenol	87-86-5	Lepomis macrochirus	4.659	2.295	3.647
220	Permethrin 3.2 EC	52645-53-1	Lepomis macrochirus	6.113	6.414	5.695
221	Phenmedipham	13684-63-4	Lepomis macrochirus	3.784	1.331	1.878
222	Phenthoate (Cidial)	2597-03-7	Lepomis macrochirus	3.924	5.227	4.987
223	Phosalone	2310-17-0	Lepomis macrochirus	4.619	2.486	3.867
224	Phosmet	732-11-6	Lepomis macrochirus	2.874	4.753	4.159
225	Phosphoric acid Divosan X-Tend formulation	7664-38-2	Lepomis macrochirus	-0.929	-0.030	0.213
226	Picoxystrobin	117428-22-5	Lepomis macrochirus	3.84	4.185	3.679
227	Piperalin	3478-94-2	Lepomis macrochirus	4.415	2.242	2.632
228	Piperonyl butoxide	51-03-6	Lepomis macrochirus	3.718	2.822	1.927
229	Prallethrin	23031-36-9	Lepomis macrochirus	3.449	4.685	4.135
230	Profenofos	41198-08-7	Lepomis macrochirus	5.769	5.604	4.294
231	Prometon	1610-18-0	Lepomis macrochirus	1.521	0.943	1.162

232	Prometryn	7287-19-6	Lepomis macrochirus	2.234	1.113	1.383
233	Propargite	2312-35-8	Lepomis macrochirus	4.517	3.675	4.053
234	Propetamphos	31218-83-4	Lepomis macrochirus	2.722	4.931	3.168
235	Propiconazole Tilt 3.6 E	60207-90-1	Lepomis macrochirus	3.653	2.029	2.420
236	Propionic acid Prothioconazole (JAU 6476 Technical)	79-09-4 178928-70-6	Lepomis macrochirus	0.481	0.514	-0.061
237	Pyraclostrobin	175013-18-0	Lepomis macrochirus	2.857	2.458	1.911
238	Pyraflufen-ethyl	129630-19-9	Lepomis macrochirus	4.239	4.393	4.532
239	Pyrethrins	8003-34-7	Lepomis macrochirus	4.076	2.735	2.098
240	Pyridaben	96489-71-3	Lepomis macrochirus	3.711	4.507	4.571
241	Pyrimethanil (radiolabeled)	53112-28-0	Lepomis macrochirus	5.242	5.838	5.161
242	Pyriproxyfen	95737-68-1	Lepomis macrochirus	2.837	1.817	0.881
243	Quinclorac	84087-01-4	Lepomis macrochirus	4.72	2.905	1.736
244	Quizalofop-ethyl	76578-14-8	Lepomis macrochirus	3.24	0.910	0.884
245	Resmethrin	10453-86-8	Lepomis macrochirus	4.406	2.003	2.909
246	Rotenone	83-79-4	Lepomis macrochirus	5.152	6.187	5.654
247	Ryanodine Ryan 50 powder Sethoxydim Poast Herbicide formulation	15662-33-6 74051-80-2	Lepomis macrochirus	3.703	5.028	4.856
248	Simazine	122-34-9	Lepomis macrochirus	-0.67	4.050	1.426
249	S-Metolachlor	87392-12-9	Lepomis macrochirus	4.502	2.100	2.311
250	Strychnine	57-24-9	Lepomis macrochirus	1.389	2.263	1.100
251	Sulfentrazone	122836-35-5	Lepomis macrochirus	3.164	1.038	1.948
252	Sulfotepp	3689-24-5	Lepomis macrochirus	2.093	1.524	2.643
253	TCMTB	21564-17-0	Lepomis macrochirus	2.416	0.807	0.616
254	Tebuconazole	107534-96-3	Lepomis macrochirus	4.364	5.110	2.952
255	Tebufenozide	112410-23-8	Lepomis macrochirus	3.56	4.015	4.436
256	Tebufenpyrad	119168-77-3	Lepomis macrochirus	3.342	2.029	1.732
257	Tebuthiuron	34014-18-1	Lepomis macrochirus	4.452	1.967	2.070
258	Tefluthrin	79538-32-2	Lepomis macrochirus	3.863	3.919	3.555
259				1.611	-0.114	0.333
260				5.552	6.777	6.508

261	Tepraloxydim (BAS 620 00 H)	149979-41-9	Lepomis macrochirus	3.739	1.665	0.642
262	Terbacil	5902-51-2	Lepomis macrochirus	0.772	0.523	0.323
263	Terbufos	13071-79-9	Lepomis macrochirus	4.889	5.969	5.574
264	Terbuthylazine	5915-41-3	Lepomis macrochirus	2.167	1.035	1.486
265	Terbutryn	886-50-0	Lepomis macrochirus	2.236	1.958	1.951
266	Tetraconazole	112281-77-3	Lepomis macrochirus	4.243	2.151	1.985
267	Tetrahydro-2(nitromethylene)-2H-1, 3-thiazine	58842-20-9	Lepomis macrochirus	0.788	0.675	0.052
268	Tetramethrin	7696-12-0	Lepomis macrochirus	2.965	3.867	4.319
269	Thiabendazole	148-79-8	Lepomis macrochirus	2.204	2.812	1.158
270	Thiacloprid	111988-49-9	Lepomis macrochirus	2.121	1.050	1.001
271	Thiazopyr	117718-60-2	Lepomis macrochirus	4.517	1.813	2.054
272	Thiobencarb	28249-77-6	Lepomis macrochirus	4.035	3.406	2.663
273	Thiodicarb	59669-26-0	Lepomis macrochirus	2.601	4.118	2.470
274	Thiophanate-methyl	23564-05-8	Lepomis macrochirus	1.792	1.810	1.324
275	Tolfenpyrad	129558-76-5	Lepomis macrochirus	4.667	5.584	5.611
276	Tolylfluanid DMST metabolite	66840-71-9	Lepomis macrochirus	1.213	0.838	0.751
277	Toxaphene (Cancelled in U.S.)	8001-35-2	Lepomis macrochirus	6.073	4.615	5.234
278	Tralomethrin	66841-25-6	Lepomis macrochirus	7.461	7.232	5.376
279	Triadimefon	43121-43-3	Lepomis macrochirus	3.124	2.230	1.468
280	Triadimenol	55219-65-3	Lepomis macrochirus	2.916	2.073	1.295
281	Triallate	2303-17-5	Lepomis macrochirus	4.844	3.525	2.370
282	Triazamate	112143-82-5	Lepomis macrochirus	1.76	4.351	2.628
283	Tributyltin fluoride(TBTF)	1983-10-4	Lepomis macrochirus	5.302	6.096	4.922
284	Tributyltin oxide	56-35-9	Lepomis macrochirus	9.695	5.553	4.997
285	Trichloromelamine	7673-09-8	Lepomis macrochirus	1.569	2.282	1.707
286	Trichloro-s-triazinetriene	87-90-1	Lepomis macrochirus	-0.823	3.136	3.065
287	Triclopyr acid	55335-06-3	Lepomis macrochirus	2.505	0.286	0.239
288	Triclopyr butoxyethyl ester (Garlon 4)	64700-56-7	Lepomis macrochirus	3.781	3.008	2.996
289	Tridiphane (DOWCO 356)	58138-08-2	Lepomis macrochirus	4.979	3.108	2.938

290	Trifloxystrobin	141517-21-7	Lepomis macrochirus	4.17	4.208	3.879
291	Triforine	26644-46-2	Lepomis macrochirus	1.489	1.191	1.253
292	Trimethacarb	2686-99-9	Lepomis macrochirus	2.33	4.031	1.809
293	Vinclozolin	50471-44-8	Lepomis macrochirus	3.421	1.894	0.780
294	Warfarin	81-81-2	Lepomis macrochirus	3.61	0.644	0.545
295	(S)-Dimethenamid	163515-14-8	Oncorhynchus mykiss	2.972	1.361	1.641
296	1,2-Benzenedicarboxaldehyde	643-79-8	Oncorhynchus mykiss	1.312	3.188	3.827
297	1,2-Benzisothiazolin-3-one	2634-33-5	Oncorhynchus mykiss	1.108	2.138	2.304
298	1,2-Benzisothiazolin-3-one, 2-butyl	4299-07-4	Oncorhynchus mykiss	2.863	3.330	3.094
299	1,3 Dichloropropene (Telone soil fumigant)	542-75-6	Oncorhynchus mykiss	1.978	3.091	2.051
300	1,3,5-Triethylhexahydro-s-triazine,VancideTH	7779-27-3	Oncorhynchus mykiss	0.838	1.049	0.866
301	2,4-D 2-EHE Selective Weed Killer	1928-43-4	Oncorhynchus mykiss	5.609	2.824	1.665
302	2,4-D Acid	94-75-7	Oncorhynchus mykiss	2.457	0.947	0.303
303	2,4-D Butoxyethanol Ester	1929-73-3	Oncorhynchus mykiss	3.732	2.276	2.694
304	2,4-D Isopropyl Ester	94-11-1	Oncorhynchus mykiss	3.324	2.005	2.581
305	2,4-D Propylene Glycol B.E. Ester	1320-18-9	Oncorhynchus mykiss	4.121	2.446	2.548
306	2,4-DB Acid	94-82-6	Oncorhynchus mykiss	3.237	0.993	2.095
307	2-Benzyl-4-chlorophenol (Nipacide BCP)	120-32-1	Oncorhynchus mykiss	3.636	2.569	2.482
308	2-Bromo-4'-hydroxyacetophenone (BHAP)	2491-38-5	Oncorhynchus mykiss	1.97	1.500	2.219
309	2-EEEBC (Debacarb)	62732-91-6	Oncorhynchus mykiss	1.683	-0.964	1.023
310	2-Hydroxyethyl octyl sulfide MGK 874 repellent	3547-33-9	Oncorhynchus mykiss	3.072	2.711	1.817
311	2-Hydroxypropyl methanethiosulfonate(HPMTS)	30388-01-3	Oncorhynchus mykiss	0.06	1.152	0.784
312	2-Methyl Benzisothiazolone(MBIT)	2527-66-4	Oncorhynchus mykiss	1.6	2.254	2.838
313	3,5 Dimethyl-1-(hydroxymethyl)pyrazole	85264-33-1	Oncorhynchus mykiss	0.45	0.600	0.011

314	3-Iodo-2-propynyl butyl carbamate (IPBC)	55406-53-6	Oncorhynchus mykiss	1.909	3.245	3.623
315	4,4-Dimethyloxazolidine	51200-87-4	Oncorhynchus mykiss	0.342	0.352	0.026
316	4,5-Dichloro-2-n-octyl-3(2H)-isothiazolone	64359-81-5	Oncorhynchus mykiss	3.709	4.733	5.019
317	4-Chloro-3,5-xylenol (Ottasept))	88-04-0	Oncorhynchus mykiss	2.662	1.763	2.639
318	4-Chloro-3-cresol	59-50-7	Oncorhynchus mykiss	2.354	1.792	2.192
319	Acetochlor WF2061 formulation	34256-82-1	Oncorhynchus mykiss	3.123	1.574	2.851
320	Acibenzolar-s-methyl	135158-54-2	Oncorhynchus mykiss	2.195	1.860	2.378
321	Alachlor	15972-60-8	Oncorhynchus mykiss	2.987	1.544	3.051
322	Aldicarb	116-06-3	Oncorhynchus mykiss	1.47	2.666	2.531
323	Ametryn	834-12-8	Oncorhynchus mykiss	1.846	0.909	1.852
324	Aminocarb	2032-59-9	Oncorhynchus mykiss	1.779	4.620	2.742
325	Aminocyclopyrachlor methyl ester	858954-83-3	Oncorhynchus mykiss	1.376	1.029	1.211
326	Amitraz	33089-61-1	Oncorhynchus mykiss	4.872	1.939	2.598
327	Anilazine	101-05-3	Oncorhynchus mykiss	3.575	2.463	3.294
328	Aspon (Ortho Sod-Cancelled in U.S.)	3244-90-4	Oncorhynchus mykiss	5.924	5.758	3.697
329	Atrazine	1912-24-9	Oncorhynchus mykiss	1.777	1.495	1.610
330	Azinphos-methyl	86-50-0	Oncorhynchus mykiss	2.382	5.448	4.557
331	Azoxystrobin	131860-33-8	Oncorhynchus mykiss	4.093	3.192	2.934
332	BCDM Hydantoin, 1-bromo-3-chloro-5,5-dimethyl	16079-88-2	Oncorhynchus mykiss	1.493	2.650	3.237
333	Bendiocarb	22781-23-3	Oncorhynchus mykiss	1.912	3.883	2.409
334	Benfluralin Balan EC formulation	1861-40-1	Oncorhynchus mykiss	4.148	2.186	3.617
335	Benomyl 50WP formulation	17804-35-2	Oncorhynchus mykiss	2.572	3.329	3.232
336	Bensulide	741-58-2	Oncorhynchus mykiss	4.423	2.836	2.742
337	Benzyl bromoacetate	5437-45-6	Oncorhynchus mykiss	2.125	2.998	3.260
338	Bethoxazin BTCN metabolite (Canceled in U.S.)	163269-30-5	Oncorhynchus mykiss	2.94	2.196	2.204
339	Bifenazate	149877-41-8	Oncorhynchus mykiss	3.824	2.779	2.597
340	Biobor JF (7.2% as boron)	2665-13-6	Oncorhynchus mykiss	1.419	-0.407	0.605

341	Bioresmethrin Bis (3-aminopropyl)dodecylamine)	28434-01-7	Oncorhynchus mykiss	5.152	5.626	5.737
342	Lonzabac 12	2372-82-9	Oncorhynchus mykiss	3.907	3.613	2.122
343	Bis (trichloromethyl) sulfone	3064-70-8	Oncorhynchus mykiss	3.057	3.240	4.016
344	Bitertanol	55179-31-2	Oncorhynchus mykiss	3.93	1.856	2.186
345	Boscalid	188425-85-6	Oncorhynchus mykiss	4.258	1.809	2.104
346	Brodifacoum	56073-10-0	Oncorhynchus mykiss	7.79	2.728	4.418
347	Bromacil	314-40-9	Oncorhynchus mykiss	1.097	0.334	0.864
348	Bromadiolone	28772-56-7	Oncorhynchus mykiss	7.184	3.342	2.576
349	Bromonitrostyrene Bromoxynil AXF 1240 formulation	7166-19-0	Oncorhynchus mykiss	2.657	3.978	3.927
350		1689-84-5	Oncorhynchus mykiss	2.789	0.573	1.187
351	Bromoxynil butyrate	3861-41-4	Oncorhynchus mykiss	3.789	3.239	4.078
352	Bromoxynil octanoate	1689-99-2	Oncorhynchus mykiss	5.349	3.549	3.605
353	Bromuconazole (EXP 10064)	116255-48-2	Oncorhynchus mykiss	3.664	3.647	2.346
354	Bronopol	52-51-7	Oncorhynchus mykiss	-0.661	2.097	1.000
355	Butralin	33629-47-9	Oncorhynchus mykiss	4.011	3.391	2.902
356	Butylate	2008-41-5	Oncorhynchus mykiss	3.372	1.233	1.986
357	Cadusafos	95465-99-9	Oncorhynchus mykiss	5.194	5.172	3.311
358	Carbendazim	10605-21-7	Oncorhynchus mykiss	1.259	3.240	3.120
359	Carbofuran	1563-66-2	Oncorhynchus mykiss	2.118	3.882	2.786
360	Carboxin	5234-68-4	Oncorhynchus mykiss	2.62	0.445	2.071
361	Chlorethoxyfos	54593-83-8	Oncorhynchus mykiss	4.619	5.914	3.577
362	Chlorfenapyr	122453-73-0	Oncorhynchus mykiss	5.455	4.718	4.739
363	Chlorflurenol methyl ester	37339-61-0	Oncorhynchus mykiss	2.729	1.564	2.374
364	Chloroneb	2675-77-6	Oncorhynchus mykiss	3.011	1.524	1.748
365	Chlorophacinone	3691-35-8	Oncorhynchus mykiss	4.736	2.944	3.172
366	Chlorpropham	101-21-3	Oncorhynchus mykiss	3.297	1.762	1.850
367	Chlorpyrifos	2921-88-2	Oncorhynchus mykiss	5.101	6.545	4.694
368	Chlorpyrifos methyl	5598-13-0	Oncorhynchus mykiss	4.321	5.463	4.408

369	Chlorthal dimethyl (DCPA or Dacthal)	1861-32-1	Oncorhynchus mykiss	3.873	1.134	1.702
370	Chromic acid	7738-94-5	Oncorhynchus mykiss	-1.354	2.191	0.625
371	Cinnamaldehyde	104-55-2	Oncorhynchus mykiss	1.899	1.273	1.898
372	Clethodim	99129-21-2	Oncorhynchus mykiss	4.844	1.251	1.277
373	Clomazone	81777-89-1	Oncorhynchus mykiss	2.64	1.664	1.101
374	Cyanamide (Alzodef)	420-04-2	Oncorhynchus mykiss	-0.574	0.798	-0.342
375	Cyanazine	21725-46-2	Oncorhynchus mykiss	1.671	0.758	1.427
376	Cyazofamid (400 SC formulation)	120116-88-3	Oncorhynchus mykiss	2.038	3.313	2.763
377	Cycloate	1134-23-2	Oncorhynchus mykiss	3.514	0.953	1.680
378	Cyflufenamid 149-F1 metabolite Cyfluthrin (Tempo 2EC Formulation)	180409-60-3 68359-37-5	Oncorhynchus mykiss	4.431 6.317	1.457 7.240	2.598 6.168
380	Cyhalothrin	68085-85-8	Oncorhynchus mykiss	6.544	6.073	5.921
381	Cyhexatin	13121-70-5	Oncorhynchus mykiss	5.927	6.355	5.475
382	Cymoxanil	57966-95-7	Oncorhynchus mykiss	-0.642	2.394	0.512
383	Cyphenothrin	39515-40-7	Oncorhynchus mykiss	5.825	5.941	6.043
384	Cyproconazole	94361-06-5	Oncorhynchus mykiss	2.865	1.050	1.186
385	Cyprodinil	121552-61-2	Oncorhynchus mykiss	3.406	3.848	1.971
386	Daminozide	1596-84-5	Oncorhynchus mykiss	-0.556	0.211	0.031
387	Dazomet	533-74-4	Oncorhynchus mykiss	0.797	2.692	3.006
388	DBDMH Glybrom formulation	77-48-5	Oncorhynchus mykiss	1.649	2.532	3.252
389	DBNPA DCDMH (Dantochlor Formulation)	10222-01-2 118-52-5	Oncorhynchus mykiss	0.481 1.337	2.449 2.622	2.384 2.335
391	DDT (Cancelled in U.S.)	50-29-3	Oncorhynchus mykiss	6.496	4.878	4.937
392	Deltamethrin	52918-63-5	Oncorhynchus mykiss	6.49	6.662	6.306
393	Desmedipham	13684-56-5	Oncorhynchus mykiss	3.866	2.203	2.247
394	Diazinon	333-41-5	Oncorhynchus mykiss	3.968	5.766	3.529
395	Dibromodicyanobutane	35691-65-7	Oncorhynchus mykiss	2.546	2.082	2.205
396	Dicamba	1918-00-9	Oncorhynchus mykiss	2.7	0.300	0.897
397	Dichlobenil	1194-65-6	Oncorhynchus mykiss	2.865	1.443	1.543

398	Dichlormid Dichlorprop (2,4-DP) Weedone formulation	37764-25-3 120-36-5	Oncorhynchus mykiss Oncorhynchus mykiss	1.991 2.845	0.169 4.647	0.169 2.672
399	Dichlorvos in Muscalure Z-9 formulation	62-73-7	Oncorhynchus mykiss	2.68	2.311	3.344
400	Diclofop-methyl	51338-27-3	Oncorhynchus mykiss	4.726	3.171	3.303
401	Dicloran (DCNA)	99-30-9	Oncorhynchus mykiss	2.484	2.000	2.568
402	Dienochlor	2227-17-0	Oncorhynchus mykiss	7.726	2.597	3.977
403	Diethyl toluamide (DEET)	134-62-3	Oncorhynchus mykiss	2.477	0.407	0.429
404	Difenoconazole	119446-68-3	Oncorhynchus mykiss	4.666	2.722	2.700
405	Difethialone	104653-34-1	Oncorhynchus mykiss	8.259	5.089	4.024
406	Diiodomethyl p-tolyl sulfone (Amical 48)	20018-09-1	Oncorhynchus mykiss	2.922	3.774	3.511
407	Dimethenamid Dimethepin (Harvade 25F formulation)	87674-68-8 55290-64-7	Oncorhynchus mykiss Oncorhynchus mykiss	2.972 0.081	1.236 1.503	2.026 0.575
408	Dinocap	39300-45-3	Oncorhynchus mykiss	5.058	4.938	4.448
409	Diphacinone	82-66-6	Oncorhynchus mykiss	4.083	2.277	2.082
410	Diphenamid	957-51-7	Oncorhynchus mykiss	2.907	0.616	0.601
411	Diphenylamine Dipropyl isocinchomeronate MGK 326 repellent	122-39-4 136-45-8	Oncorhynchus mykiss Oncorhynchus mykiss	3.43 2.215	2.149 1.145	1.886 2.400
412	Dithiopyr Dimension formulation	97886-45-8	Oncorhynchus mykiss	5.243	1.888	2.941
413	Diuron Karmex DF Formulation	330-54-1	Oncorhynchus mykiss	3.087	1.443	2.077
414	D-Phenothrin (Sumithrin)	26002-80-2	Oncorhynchus mykiss	5.761	4.901	5.398
415	DTEA	36362-09-1	Oncorhynchus mykiss	3.819	3.781	2.451
416	d-trans-Allethrin	584-79-2	Oncorhynchus mykiss	4.002	4.531	4.494
417	Endothall	145-73-3	Oncorhynchus mykiss	-0.051	0.758	2.015
418	Esfenvalerate Ethalfuralin Sonalan EC formulation	66230-04-4 55283-68-6	Oncorhynchus mykiss Oncorhynchus mykiss	6.68 3.924	6.447 4.265	6.778 3.955
419	Ethephon	16672-87-0	Oncorhynchus mykiss	0.403	0.659	0.081
420	Ethofenprox	80844-07-1	Oncorhynchus mykiss	6.372	5.820	5.430

425	Ethoprop	13194-48-4	Oncorhynchus mykiss	4.417	3.753	2.324
426	Ethoxyquin	91-53-2	Oncorhynchus mykiss	3.693	2.036	1.082
427	Ethyl N,N-dipropylthiocarbamate (EPTC)	759-94-4	Oncorhynchus mykiss	2.982	1.128	0.977
428	Farnesol	4602-84-0	Oncorhynchus mykiss	4.398	2.005	2.092
429	Fenamidone(RPA413255 s-enantiomer)	161326-34-7	Oncorhynchus mykiss	3.49	1.507	2.624
430	Fenamiphos NemaCur 3 formulation	22224-92-6	Oncorhynchus mykiss	4.238	5.368	3.624
431	Fenarimol	60168-88-9	Oncorhynchus mykiss	4.068	1.688	2.198
432	Fenazaquin	120928-09-8	Oncorhynchus mykiss	4.549	4.738	3.154
433	Fenbuconazole	114369-43-6	Oncorhynchus mykiss	4.026	2.166	2.351
434	Fenbutatin oxide	13356-08-6	Oncorhynchus mykiss	16.761	4.531	5.792
435	Fenhexamid	126833-17-8	Oncorhynchus mykiss	4.608	0.459	2.353
436	Fenoxaprop-ethyl	66441-23-4	Oncorhynchus mykiss	4.604	2.056	2.030
437	Fenoxycarb	72490-01-8	Oncorhynchus mykiss	3.604	2.877	2.660
438	Fenpropathrin	39515-41-8	Oncorhynchus mykiss	5.269	5.819	5.182
439	Fenpropimorph	67564-91-4	Oncorhynchus mykiss	4.272	2.106	1.943
440	Fenpyrazamine	473798-59-3	Oncorhynchus mykiss	3.676	1.780	1.804
441	Fenpyroximate FujiMite 5EC	134098-61-6	Oncorhynchus mykiss	5.027	5.421	5.854
442	Fenthion	55-38-9	Oncorhynchus mykiss	3.996	4.729	2.704
443	Fenvalerate	51630-58-1	Oncorhynchus mykiss	6.68	6.924	6.208
444	Fipronil MB 46136 metabolite	120068-37-3	Oncorhynchus mykiss	4.877	4.178	4.149
445	Flazasulfuron DTPU Degradate	104040-78-0	Oncorhynchus mykiss	-0.236	0.390	0.549
446	Fluazifop-butyl (PP009)	69806-50-4	Oncorhynchus mykiss	5.003	1.804	1.893
447	Fluazinam	79622-59-6	Oncorhynchus mykiss	5.986	3.412	4.111
448	Fludioxonil(Maxim 4FS)	131341-86-1	Oncorhynchus mykiss	2.393	2.441	2.723
449	Flumioxazin	103361-09-7	Oncorhynchus mykiss	1.928	1.809	2.188
450	Fluometuron	2164-17-2	Oncorhynchus mykiss	2.799	1.370	1.895
451	Fluoxastrobin	361377-29-9	Oncorhynchus mykiss	4.565	2.980	3.023
452	Fluridone	59756-60-4	Oncorhynchus mykiss	4.738	2.040	1.894
453	Flurprimidol	56425-91-3	Oncorhynchus mykiss	3.267	1.482	1.295

454	Flutriafol 125 g/L SC formulation	76674-21-0	Oncorhynchus mykiss	2.492	1.631	1.587
455	Fluvalinate	69409-94-5	Oncorhynchus mykiss	7.396	6.099	5.359
456	Fluxapyroxad	907204-31-3	Oncorhynchus mykiss	4.694	1.750	2.796
457	Fonofos	944-22-9	Oncorhynchus mykiss	4.528	5.082	4.090
458	Forchlorfenuron	68157-60-8	Oncorhynchus mykiss	3.379	1.670	1.430
459	Fosthiazate	98886-44-3	Oncorhynchus mykiss	3.832	3.037	1.561
460	Furfural	98-01-1	Oncorhynchus mykiss	1.092	0.673	1.497
461	Gamma cyhalothrin	76703-62-3	Oncorhynchus mykiss	6.544	7.000	6.796
462	Glutaraldehyde	111-30-8	Oncorhynchus mykiss	0.554	2.125	1.023
463	Grotan	4719-04-4	Oncorhynchus mykiss	-2.245	0.924	0.718
464	Hexaconazole JF 9445 formulation - test 1	79983-71-4	Oncorhynchus mykiss	3.663	2.218	1.917
465	Hexazinone	51235-04-2	Oncorhynchus mykiss	0.513	0.473	0.236
466	Hydramethylnon	67485-29-4	Oncorhynchus mykiss	6.382	2.637	3.518
467	Imazalil	35554-44-0	Oncorhynchus mykiss	4.134	1.973	2.303
468	Imazamethabenz	81405-85-8	Oncorhynchus mykiss	2.073	0.117	0.013
469	Imazaquin	81335-37-7	Oncorhynchus mykiss	2.224	0.046	0.046
470	Imidacloprid	138261-41-3	Oncorhynchus mykiss	0.383	0.477	0.048
471	Imiprothrin (Pralle)	72963-72-5	Oncorhynchus mykiss	1.623	3.795	3.923
472	Indoxacarb IN-MP819	173584-44-6	Oncorhynchus mykiss	4.093	3.916	4.342
473	Inert Surfadone(LP100)	2687-94-7	Oncorhynchus mykiss	1.706	1.299	0.929
474	Ipconazole	125225-28-7	Oncorhynchus mykiss	3.588	2.293	2.339
475	Iprodione	36734-19-7	Oncorhynchus mykiss	2.88	3.139	1.895
476	Irgarol	28159-98-0	Oncorhynchus mykiss	2.378	1.679	2.529
477	Isazophos methyl Triumph 4E formulation	42509-83-1	Oncorhynchus mykiss	2.791	5.113	4.652
478	Isopropalin	33820-53-0	Oncorhynchus mykiss	4.253	3.061	2.586
479	Kepone (Cancelled in U.S.)	143-50-0	Oncorhynchus mykiss	4.823	3.276	4.329
480	Kresoxim methyl	143390-89-0	Oncorhynchus mykiss	2.611	2.975	3.217
481	Lactofen	77501-63-4	Oncorhynchus mykiss	5.168	2.363	2.096
482	Lambda-Cyhalothrin	91465-08-6	Oncorhynchus mykiss	6.544	7.051	6.374

483	Limonene	138-86-3	Oncorhynchus mykiss	3.309	0.543	0.231
484	Linalool	78-70-6	Oncorhynchus mykiss	2.67	0.624	0.729
485	Linuron	330-55-2	Oncorhynchus mykiss	3.019	3.317	1.907
486	L-Lactic acid	79-33-4	Oncorhynchus mykiss	-0.548	-0.920	-0.159
487	Malathion	121-75-5	Oncorhynchus mykiss	2.505	5.519	4.906
488	Maleic hydrazide	123-33-1	Oncorhynchus mykiss	-1.901	0.018	-1.107
489	Mandipropamid	374726-62-2	Oncorhynchus mykiss	3.41	1.764	1.971
490	MCPA 2-ethylhexyl ester	29450-45-1	Oncorhynchus mykiss	4.787	3.048	1.990
491	Mefenpyr diethyl	135590-91-9	Oncorhynchus mykiss	3.444	1.824	1.949
492	Mesotrione(MNBA metabolite)	104206-82-8	Oncorhynchus mykiss	1.119	0.404	0.355
493	Metaflumizone 320 I formulation	139968-49-3	Oncorhynchus mykiss	6.244	2.296	2.840
494	Metalaxyl Ridomil 2E-G	57837-19-1	Oncorhynchus mykiss	1.844	1.349	1.181
495	Metconazole (cis/trans isomers)	125116-23-6	Oncorhynchus mykiss	3.342	1.734	1.773
496	Methamidophos	10265-92-6	Oncorhynchus mykiss	1.063	3.735	2.042
497	Methidathion	950-37-8	Oncorhynchus mykiss	1.904	4.674	4.480
498	Methomyl	16752-77-5	Oncorhynchus mykiss	1.039	4.266	2.276
499	Methoprene	40596-69-8	Oncorhynchus mykiss	5.062	2.543	2.488
500	Methyl anthralinate	134-20-3	Oncorhynchus mykiss	1.055	0.919	0.820
501	Methyl isothiocyanate	556-61-6	Oncorhynchus mykiss	0.719	2.983	3.155
502	Methyl nonyl ketone	112-12-9	Oncorhynchus mykiss	3.716	2.499	1.754
503	Methylisothiazolinone (Kathon OM formulation)	2682-20-4	Oncorhynchus mykiss	0.447	2.806	3.216
504	Metofluthrin	240494-70-6	Oncorhynchus mykiss	4.281	4.885	5.478
505	Metolachlor CGA-51502 Metrafenone CL 4084564 metabolite	51218-45-2	Oncorhynchus mykiss	3.164	1.265	1.862
506		220899-03-6	Oncorhynchus mykiss	4.331	0.905	1.413
507	Metribuzin	21087-64-9	Oncorhynchus mykiss	0.372	1.710	0.708
508	MGK-264	113-48-4	Oncorhynchus mykiss	3.006	2.078	3.213
509	Mirex (Cancelled in U.S.)	2385-85-5	Oncorhynchus mykiss	7.664	2.442	4.375
510	Mitin FF	3567-25-7	Oncorhynchus mykiss	6.983	1.742	1.885
511	MTI	82633-79-2	Oncorhynchus mykiss	0.935	2.077	2.242

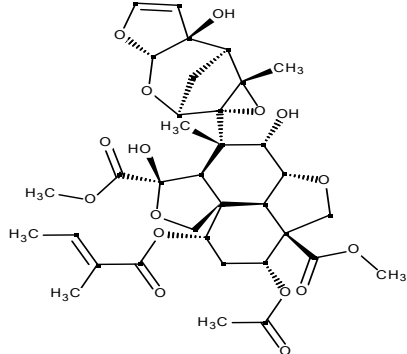
512	Myclobutanil	88671-89-0	Oncorhynchus mykiss	3.583	1.419	1.837
513	N6-Benzyladenine	1214-39-7	Oncorhynchus mykiss	1.435	1.041	1.022
514	Naled	300-76-5	Oncorhynchus mykiss	3.651	6.104	3.467
515	Naphthalene	91-20-3	Oncorhynchus mykiss	2.84	1.904	1.807
516	Naphthaleneacetic acid	86-87-3	Oncorhynchus mykiss	2.467	0.015	1.124
517	Napropamide	15299-99-7	Oncorhynchus mykiss	3.476	1.278	1.460
518	Neurolidol	7212-44-4	Oncorhynchus mykiss	3.197	2.237	2.324
519	Niclosamide	1420-04-8	Oncorhynchus mykiss	3.86	3.214	4.100
520	Nitrapyrin	1929-82-4	Oncorhynchus mykiss	3.562	2.021	2.002
521	N-Methyl-2-pyrrolidine N-methylneodecanamide	120-94-5	Oncorhynchus mykiss	0.712	-1.769	-1.554
522	(MNDA)	105726-67-8	Oncorhynchus mykiss	2.729	0.154	0.411
523	Nonanoic acid	112-05-0	Oncorhynchus mykiss	2.822	0.217	0.240
524	OBPA	58-36-6	Oncorhynchus mykiss	2.826	5.020	5.157
525	Octhilinone	26530-20-1	Oncorhynchus mykiss	2.576	3.300	3.657
526	Ortho-phenyl phenol	90-43-7	Oncorhynchus mykiss	3.059	1.831	1.792
527	Oryzalin	19044-88-3	Oncorhynchus mykiss	1.777	2.363	2.026
528	Oxadiazon	19666-30-9	Oncorhynchus mykiss	4.217	2.814	2.517
529	Oxamyl	23135-22-0	Oncorhynchus mykiss	0.107	2.669	1.773
530	Oxazolidine E	7747-35-5	Oncorhynchus mykiss	0.413	0.533	-0.188
531	Oxycarboxin	5259-88-1	Oncorhynchus mykiss	1.302	0.588	1.128
532	Oxydemeton-methyl	301-12-2	Oncorhynchus mykiss	2.487	3.187	2.528
533	Oxyfluorfen	42874-03-3	Oncorhynchus mykiss	5.458	3.655	3.160
534	Oxythioquinox	2439-01-2	Oncorhynchus mykiss	2.575	3.291	3.263
535	Paclobutrazol	76738-62-0	Oncorhynchus mykiss	3.122	0.947	1.024
536	Paranitrophenol	100-02-7	Oncorhynchus mykiss	1.3	1.365	1.490
537	Pebulate	1114-71-2	Oncorhynchus mykiss	3.372	1.474	1.439
538	Pendimethalin	40487-42-1	Oncorhynchus mykiss	3.72	3.002	3.309
539	Pentachloronitrobenzene (PCNB)	82-68-8	Oncorhynchus mykiss	4.862	2.584	2.979
540	Pentachlorophenol	87-86-5	Oncorhynchus mykiss	4.659	2.295	3.550
541	Penthiopyrad 20 SC formulation	183675-82-3	Oncorhynchus mykiss	4.902	3.094	2.969

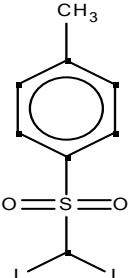
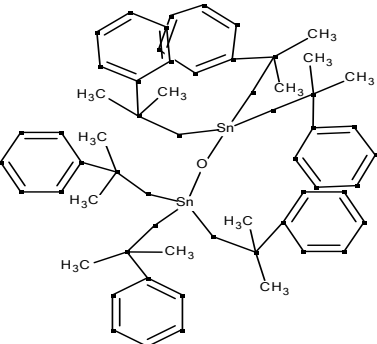
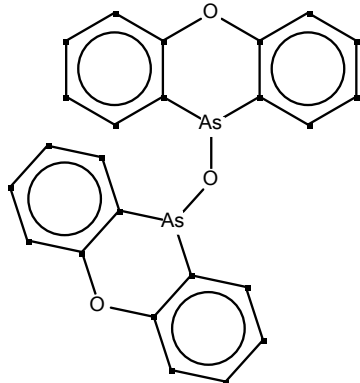
542	Permethrin 3.2 EC	52645-53-1	Oncorhynchus mykiss	6.113	6.414	5.270
543	Phenmedipham	13684-63-4	Oncorhynchus mykiss	3.784	1.331	2.328
544	Phenthoate (Cidial)	2597-03-7	Oncorhynchus mykiss	3.924	5.227	4.426
545	Phosalone	2310-17-0	Oncorhynchus mykiss	4.619	2.486	2.766
546	Phosmet	732-11-6	Oncorhynchus mykiss	2.874	4.753	3.480
547	Phosphoric acid Divosan X-Tend formulation	7664-38-2	Oncorhynchus mykiss	-0.929	-0.030	0.052
548	Picoxystrobin	117428-22-5	Oncorhynchus mykiss	3.84	4.185	3.720
549	Pinoxaden 100 EC formulation	243973-20-8	Oncorhynchus mykiss	3.732	2.291	2.232
550	Piperonyl butoxide	51-03-6	Oncorhynchus mykiss	3.718	2.822	2.274
551	Prallethrin	23031-36-9	Oncorhynchus mykiss	3.449	4.685	4.399
552	Profenofos	41198-08-7	Oncorhynchus mykiss	5.769	5.604	4.250
553	Prometryn	7287-19-6	Oncorhynchus mykiss	2.234	1.113	1.920
554	Propachlor	1918-16-7	Oncorhynchus mykiss	2.667	1.487	3.095
555	Propargite	2312-35-8	Oncorhynchus mykiss	4.517	3.675	3.473
556	Propiconazole Tilt 3.6 E	60207-90-1	Oncorhynchus mykiss	3.653	2.029	2.605
557	Propionic acid	79-09-4	Oncorhynchus mykiss	0.481	0.514	0.162
558	Prothioconazole (JAU 6476 Technical)	178928-70-6	Oncorhynchus mykiss	2.857	2.458	2.309
559	Pyraclostrobin	175013-18-0	Oncorhynchus mykiss	4.239	4.393	4.796
560	Pyraflufen-ethyl	129630-19-9	Oncorhynchus mykiss	4.076	2.735	2.412
561	Pyrethrins	8003-34-7	Oncorhynchus mykiss	3.711	4.507	4.864
562	Pyridaben	96489-71-3	Oncorhynchus mykiss	5.242	5.838	5.705
563	Pyridalyl	179101-81-6	Oncorhynchus mykiss	6.953	3.135	2.992
564	Pyriproxyfen	95737-68-1	Oncorhynchus mykiss	4.72	2.905	2.854
565	Quinoxifen	124495-18-7	Oncorhynchus mykiss	5.473	3.530	3.057
566	Quinalofop-ethyl	76578-14-8	Oncorhynchus mykiss	4.406	2.003	2.632
567	Resmethrin	10453-86-8	Oncorhynchus mykiss	5.152	6.187	6.082
568	Rotenone	83-79-4	Oncorhynchus mykiss	3.703	5.028	5.317
569	Ryanodine Ryan 50 powder	15662-33-6	Oncorhynchus mykiss	-0.67	4.050	2.188
570	Sedaxane SYN524464 (trans + cis isomers)	874967-67-6	Oncorhynchus mykiss	4.124	1.745	2.520

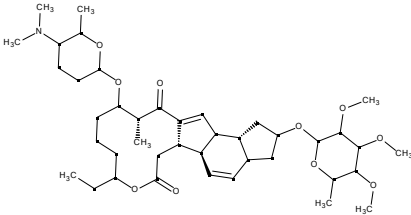
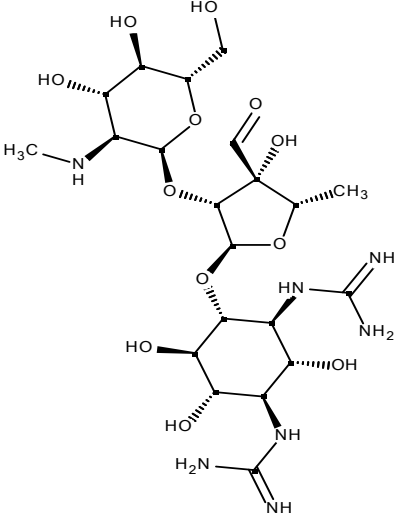
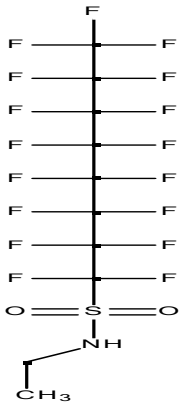
Sethoxydim Poast Herbicide						
571	formulation	74051-80-2	Oncorhynchus mykiss	4.502	2.100	2.436
572	Simazine	122-34-9	Oncorhynchus mykiss	1.389	2.263	0.697
573	S-Metolachlor	87392-12-9	Oncorhynchus mykiss	3.164	1.038	1.377
574	Strychnine	57-24-9	Oncorhynchus mykiss	2.093	1.524	2.163
575	TCMTB	21564-17-0	Oncorhynchus mykiss	3.56	4.015	4.074
576	Tebuconazole	107534-96-3	Oncorhynchus mykiss	3.342	2.029	1.845
577	Tebufenozide	112410-23-8	Oncorhynchus mykiss	4.452	1.967	1.816
578	Tebufenpyrad	119168-77-3	Oncorhynchus mykiss	3.863	3.919	4.273
579	Tebuthiuron	34014-18-1	Oncorhynchus mykiss	1.611	-0.114	0.203
580	Tefluthrin	79538-32-2	Oncorhynchus mykiss	5.552	6.777	6.844
581	Tepraloxydim (BAS 620 00 H)	149979-41-9	Oncorhynchus mykiss	3.739	1.665	1.885
582	Terbacil	5902-51-2	Oncorhynchus mykiss	0.772	0.523	0.671
583	Terbufos	13071-79-9	Oncorhynchus mykiss	4.889	5.969	4.579
584	Terbutylazine	5915-41-3	Oncorhynchus mykiss	2.167	1.035	1.830
585	Terbutryn	886-50-0	Oncorhynchus mykiss	2.236	1.958	2.469
586	Tetraconazole	112281-77-3	Oncorhynchus mykiss	4.243	2.151	1.979
587	Tetrahydro-2(nitromethylene)-2H-1, 3-thiazine	58842-20-9	Oncorhynchus mykiss	0.788	0.675	0.136
588	Thiabendazole	148-79-8	Oncorhynchus mykiss	2.204	2.812	2.556
589	Thiacloprid	111988-49-9	Oncorhynchus mykiss	2.121	1.050	0.923
590	Thiazopyr	117718-60-2	Oncorhynchus mykiss	4.517	1.813	2.067
591	Thidiazuron	51707-55-2	Oncorhynchus mykiss	2.182	1.587	1.523
592	Thiobencarb	28249-77-6	Oncorhynchus mykiss	4.035	3.406	2.390
593	Thiodicarb	59669-26-0	Oncorhynchus mykiss	2.601	4.118	2.012
594	Thiophanate-methyl	23564-05-8	Oncorhynchus mykiss	1.792	1.810	1.626
595	Tolclofos-methyl	57018-04-9	Oncorhynchus mykiss	4.581	0.798	2.640
596	Tolyfluanid	731-27-1	Oncorhynchus mykiss	3.314	3.262	4.064
597	Toxaphene (Cancelled in U.S.)	8001-35-2	Oncorhynchus mykiss	6.073	4.615	5.359
598	Tralomethrin	66841-25-6	Oncorhynchus mykiss	7.461	7.232	5.619
599	Triadimefon	43121-43-3	Oncorhynchus mykiss	3.124	2.230	1.855

600	Triadimenol	55219-65-3	Oncorhynchus mykiss	2.916	2.073	1.325
601	Triallate	2303-17-5	Oncorhynchus mykiss	4.844	3.525	2.405
602	Triazamate	112143-82-5	Oncorhynchus mykiss	1.76	4.351	2.773
603	Tributyltin fluoride(TBTF)	1983-10-4	Oncorhynchus mykiss	5.302	6.096	4.959
604	Tributyltin oxide	56-35-9	Oncorhynchus mykiss	9.695	5.553	5.027
605	Trichloromelamine	7673-09-8	Oncorhynchus mykiss	1.569	2.282	2.060
606	Triclopyr acid Triclopyr butoxyethyl ester	55335-06-3	Oncorhynchus mykiss	2.505	0.286	0.341
607	(Garlon 4)	64700-56-7	Oncorhynchus mykiss	3.781	3.008	2.739
608	Tridiphane (DOWCO 356)	58138-08-2	Oncorhynchus mykiss	4.979	3.108	2.781
609	Trifloxystrobin	141517-21-7	Oncorhynchus mykiss	4.17	4.208	4.465
610	Triforine	26644-46-2	Oncorhynchus mykiss	1.489	1.191	1.308
611	Trimethacarb	2686-99-9	Oncorhynchus mykiss	2.33	4.031	2.286
612	Vinclozolin	50471-44-8	Oncorhynchus mykiss	3.421	1.894	2.003

Table S3: List of out of AD compounds in QSTR and QSAAR models by leverage approach

S.No.	Model	Chemical name	Chemical structure
High leverage compounds			
1.	L-QSTR G-QSTR	Azadirachtin	

2.	L-QSTR	Diiodomethyl p-tolylsulfone)	
3.	L-QSTR G-QSTR	Fenbutatin oxide	
4.	L-QSTR G-QSTR	OBPA	

5.	L-QSTR	Spinosyn Factor D metabolite	 <p>The structure shows a complex polycyclic molecule with a central fused ring system, including a decalin core. It features several side chains, including a piperidine ring with a methyl group, and a sugar moiety with multiple methoxy groups.</p>
6.	L-QSTR G-QSTR	Streptomycin	 <p>The structure depicts the aminoglycoside Streptomycin, consisting of a streptidine ring linked to a 2-deoxystreptose sugar, which is further linked to a 2-amino-2-deoxyribose sugar. The streptidine ring has a methyl group on the nitrogen, and the 2-amino-2-deoxyribose has an amino group.</p>
7.	L-QSTR G-QSTR	Sulfluramid	 <p>The structure shows Sulfluramid, a perfluorinated sulfonamide. It features a central sulfur atom double-bonded to two oxygen atoms and single-bonded to a nitrogen atom. The nitrogen atom is bonded to a methyl group and a perfluorinated ethyl chain (two carbons, each with two fluorine atoms).</p>

8.	L-QSTR G-QSTR QSAAR	Tributyltin oxide	
9.	L-QSTR	DBNPA	
10.	G-QSTR	Temephos Abate 4E formulation	
High standardized residual compounds			
10.	L-QSTR G-QSTR	Dichlorprop (2,4-DP)	

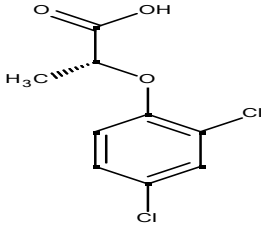
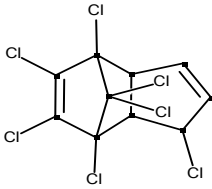
11.	L-QSTR G-QSTR	Dichlorprop P (2,4-DP-p)	
12	G-QSTR	Heptachlor	

Table S4: List of out of AD compounds in QSTR and ISC QSAAR models by standardization approach

L-QSTR Model		G-QSTR model		ISC QSAAR model	
Data set	Chemical name	Data set	Chemical name	Data set/species	Chemical name
Training	Aspon	Training	Azadirachtin	Training (<i>L. macrochirus</i>)	Brodifacoum
Training	Azadirachtin	Training	Chlorethoxyfos	Training (<i>L. macrochirus</i>)	Dienochlor
Training	Bis (trichloromethyl) sulfone	Training	Chromic acid	Training (<i>L. macrochirus</i>)	Fenbutatin oxide
Training	Chlorethoxyfos	Training	Ethion	Test (<i>L. macrochirus</i>)	Tributyltin oxide
Training	Diiodomethyl p-tolyl sulfone (Amical 48)	Training	Fenbutatin oxide	Training (<i>O. mykiss</i>)	Brodifacoum
Training	Ethion	Training	OBPA	Training (<i>O. mykiss</i>)	Cyfluthrin (Tempo 2EC Formulation)

Training	Fenbutatin oxide	Training	Phosphoric acid Divosan X-Tend formulation	Training (<i>O. mykiss</i>)	Dienochlor
Training	Naled	Training	Streptomycin	Training (<i>O. mykiss</i>)	Fenbutatin oxide
Training	OBPA	Training	Sulfluramid	Test (<i>O. mykiss</i>)	Mirex (Cancelled in U.S.)
Training	Ryanodine Ryan 50 powder	Training	Temephos Abate 4E formulation	Test (<i>O. mykiss</i>)	Tributyltin oxide
Training	Spinosyn Factor D metabolite	Training	Tributyltin oxide		
Training	Streptomycin	Training	Tris(hydroxymethyl)n itromethane		
Training	Sulfluramid	Training	Glyphosine (Polaris formula)		
Training	Temephos Abate 4E formulation	Test	Aspon (Ortho Sod- Cancelled in U.S.)		
Training	Tributyltin oxide	Test	Bis (trichloromethyl) sulfone		
Test	DBNPA	Test	Malathion		
Test	Sulfotepp	Test	Sulfotepp		
Test	Tricosene				
Test	Maneb 80WP				

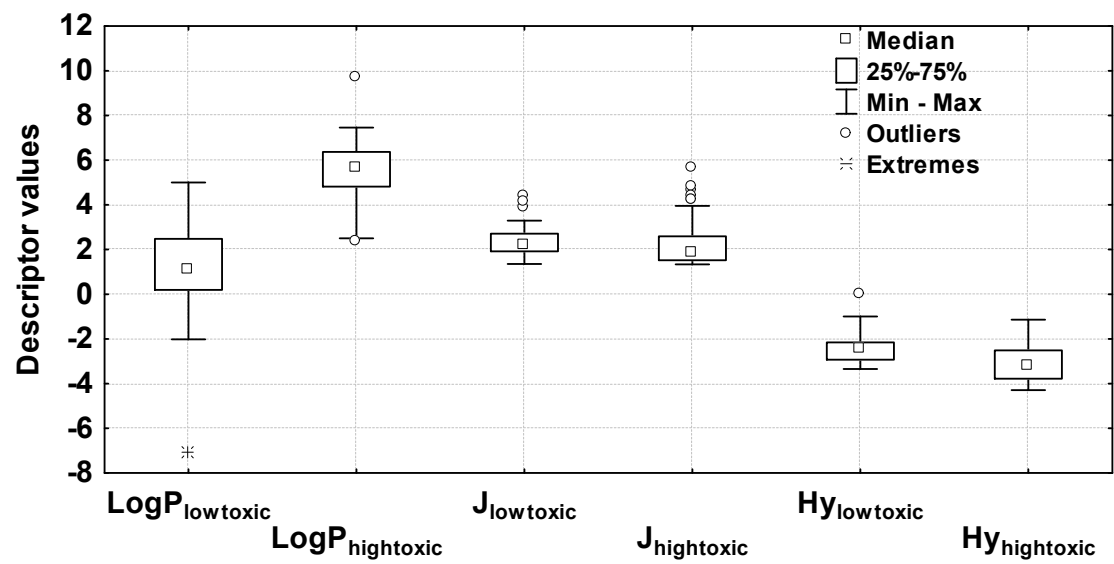


Figure S1a: Box- Whisker plot of the MDs (LogP, J, and Hy) in *D. magna* data

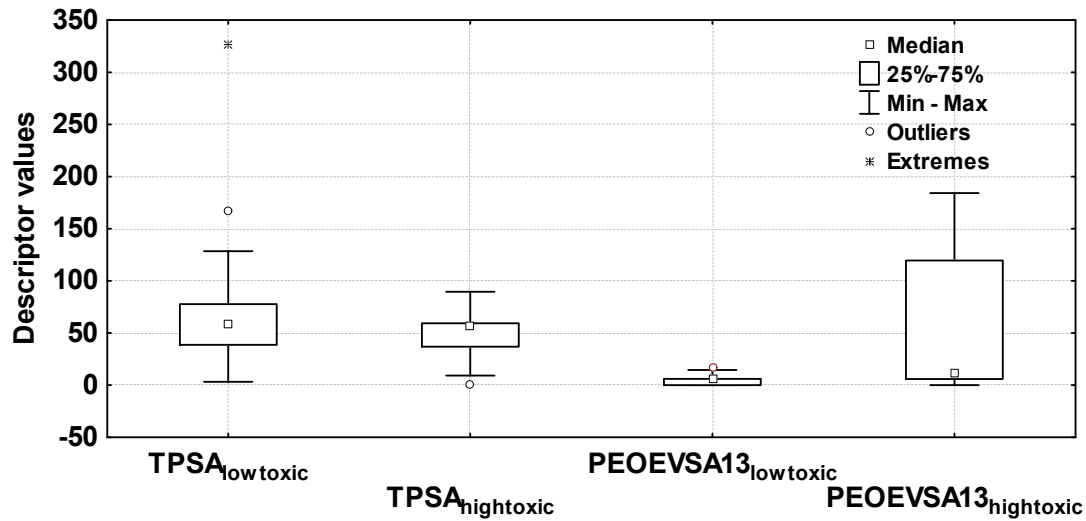


Figure S1b: Box- Whisker plot of the MDs (TPSA and PEOEVSA13) in *D. magna* data

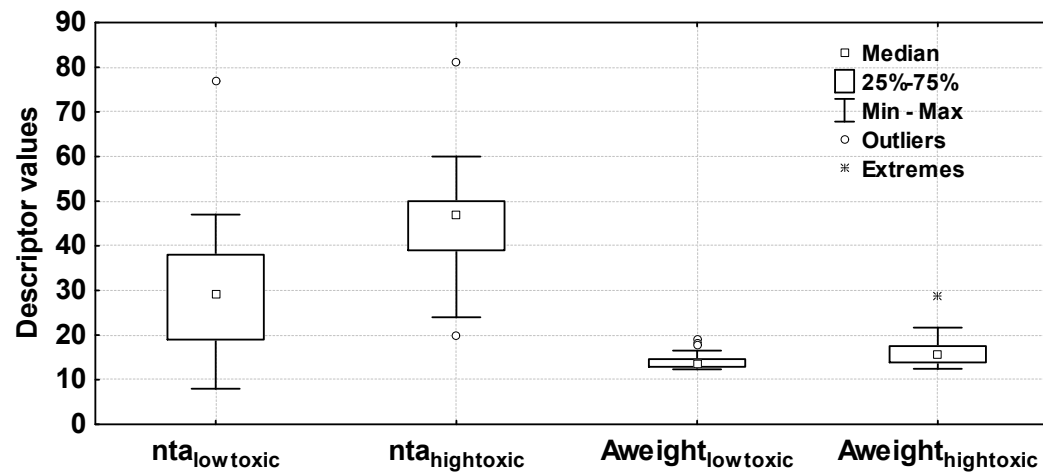


Figure S1c: Box- Whisker plot of the MDs (nta and Aweight) in *D. magna* data