Supplementary Information (SI) for Environmental Science: Processes & Impacts.

Supplementary Materials of the Manuscript:

Predictive Modelling of Pesticide Properties for Risk Assessment: A Curated Dataset and QSAR Evaluation for 110 Active Ingredients

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Table S1: Literature Derived Values (LDVs) at 25°C for pesticides active ingredients

No.	Pesticide active ingredient	CASRN	pKa	log $K_{OW,neutral}$	log $K_{AW,neutral}$	Log K_{OA}	Log K_{OC}	V_P (Pa)	S_W (mol/m³)	Solubility in Octanol (mol/m³)
1.	2,4-Dichlorophenoxyacetic acid	94-75-7	3.4	2.81	-8.65	11.46	1.66	1.70E-05	3.09E+00	
2.	Abamectin	71751-41-2	ND	4.40	-6.94	11.34	3.5[2*]	2.00E-07	6.99E-04	
3.	Acetamiprid	135410-20-7	0.7	0.74	-10.42	11.16	2.30	1.77E-06	1.89E+01	
4.	Alachlor	15972-60-8	0.62	3.52	-5.60	9.12	2.28	5.48E-03	8.90E-01	

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[2] The reported value is for avermectin B1a. Abamectin is a mixture composed mainly of avermectin B1a (>80%) and a smaller fraction of avermectin B1b (<20%). Although the two homologues differ only by one CH2 unit, this structural difference may influence sorption and other physicochemical properties. Here, we use regulatory sorption data reported for avermectin B1a as the best available empirical anchor for abamectin, while noting that component-specific uncertainty remains within the mixture

* Values inferred from non-linear Freundlich isotherms rather than directly measured linear K_{OC} value.

5.	Aldrin	309-00-2	ND	6.50	-1.12	7.62	4.69	1.60E-02	8.49E-05	
6.	Ametryn	834-12-8	10.07	2.98	-6.84	9.82	2.59	3.65E-04	1.01E+00	
7.	Atrazine	1912-24-9	1.7	2.61	-6.99	9.60	2.24	3.85E-05	1.53E-01	
8.	Azoxystrobin	131860-33-8	ND	2.50	-11.53	14.03	2.77	1.10E-10	1.49E-02	
9.	Benalaxyl	71626-11-4	ND	3.40	-5.33	8.73	3.54	1.33E-03	1.14E-01	
10.	Bentazon	25057-89-0	3.51	2.34	-7.20	9.54	1.52	3.24E-04	2.08E+00	
11.	beta-Hexachlorocyclohexane (β-HCH)	319-85-7	ND	4.14	-4.17	8.31	3.04	4.69E-03	2.78E-02	
12.	Bifenthrin	82657-04-3	ND	6.00	-2.45	8.45	5.35	2.40E-05	2.71E-06	
13.	Bitertanol	55179-31-2	ND	4.16	-10.79	14.95	3.87*	5.25E-10	1.29E-02	1.57E+02
14.	Boscalid	188425-85-6	ND	2.96	-7.30	10.26	3.43*	1.68E-06	1.34E-02	2.91E+01
15.	Brodifacoum	56073-10-0	ND	8.50	-3.82	12.32	3.96	3.15E-06	8.33E-06	
16.	Butachlor	23184-66-9	ND	4.50	-5.67	10.17	2.86	3.87E-04	7.36E-02	
17.	Cadusafos	95465-99-9	ND	3.90	-4.27	8.17	2.4*	1.20E-01	9.06E-01	
18.	Captan	133-06-2	ND	2.80	-6.54	9.34	2.30	1.20E-05	1.70E-02	
19.	Carbaryl (1-naphthyl N-methylcarbamate)	63-25-2	10.4	2.36	-6.87	9.23	2.40	1.81E-04	5.47E-01	
20.	Carbendazim	10605-21-7	4.2	1.52	-9.29	10.81	2.35	1.93E-07	1.52E-01	
21.	Carbofuran	1563-66-2	ND	2.32	-7.39	9.71	1.75	1.47E-04	1.45E+00	
22.	Chlorothalonil	1897-45-6	ND	2.90	-5.00	7.90	3.26	7.60E-05	3.05E-03	
23.	Chlorotoluron	15545-48-9	ND	2.41	-8.03	10.44	2.02	9.40E-06	4.10E-01	
24.	Chlorpyrifos	2921-88-2	ND	4.96	-3.50	8.46	3.70	2.69E-03	3.44E-03	
25.	Clethodim	99129-21-2	4.47	1.44	-8.83	10.27	1.72*	6.34E-05	1.74E+01	
26.	Cyanazine	21725-46-2	12.9	2.22	-9.61	11.83	2.28	4.32E-07	7.06E-01	
27.	Cymoxanil	57966-95-7	9.3	0.59	-7.87	8.46	2.09	1.51E-04	4.52E+00	
28.	Cypermethrin	52315-07-8	ND	6.94	-4.64	11.58	5.00	1.56E-05	2.76E-04	
29.	Cyphenothrin	39515-40-7	ND	6.29	-2.47	8.76	3.96	2.58E-04	3.06E-05	
30.	DDT (p,p'-DDT)	50-29-3	ND	6.91	-3.68	10.59	5.31	4.15E-05	8.09E-05	
31.	Deltamethrin	52918-63-5	ND	6.20	-3.69	9.89	7.01	2.00E-06	3.96E-06	
32.	Diazinon	333-41-5	2.6	3.81	-4.67	8.48	2.75	1.20E-02	2.26E-01	
33.	Dieldrin	60-57-1	ND	5.20	-3.34	8.54	4.08	7.41E-04	6.56E-04	
34.	Difenoconazole	119446-68-3	1.07	4.30	-9.44	13.74	4.15*	3.33E-08	3.69E-02	
35.	Dimethoate	60-51-5	ND	0.78	-8.00	8.78	1.20	2.51E-03	1.02E+02	
36.	Dimethomorph	110488-70-5	-1.3	2.68	-8.50	11.18	3.18*	9.85E-07	1.27E-01	

37.	Diuron	330-54-1	ND	2.68	-7.69	10.37	2.4	9.20E-06	1.80E-01	
38.	Emamectin-benzoate	155569-91-8	4.2	4.94	-6.08	11.02	5.58	2.86E-05	1.38E-02	2.40E+01
39.	Endosulfan	115-29-7	ND	3.83	-3.27	7.10	4.09	1.48E-03	1.11E-03	
40.	Endrin	72-20-8	ND	5.20	-3.39	8.59	4.08	7.24E-04	7.23E-04	
41.	Epoxiconazole	133855-98-8	ND	3.44	-7.83	11.27	3.51*	7.44E-07	2.01E-02	
42.	Ethoprophos	13194-48-4	ND	3.59	-5.18	8.77	1.85	5.07E-02	3.10E+00	
43.	Fenamiphos	22224-92-6	ND	3.23	-7.37	10.60	2.51	1.39E-04	1.32E+00	
44.	Fenbuconazole	114369-43-6	ND	3.23	-5.15	8.38	3.65*	1.05E-05	5.94E-04	
45.	Fenoxycarb	72490-01-8	ND	4.30	-7.79	12.09	3.00	8.00E-07	1.99E-02	
46.	Fenpropimorph	67564-91-4	6.98	4.93	-3.79	8.72	3.44*	6.64E-03	1.63E-02	
47.	Fipronil	120068-37-3	ND	4.00	-7.46	11.46	3.06*	3.71E-07	4.35E-03	
48.	Glufosinate	51276-47-2	2	-4.02			2.78*	1.21E-09		
49.	Glyphosate	1071-83-6	2.34	-5.40	-11.78	6.38	3.15	2.56E-05	6.21E+03	
50.	Heptachlor	76-44-8	ND	5.47	-1.35	6.82	4.38	5.33E-02	4.82E-04	
51.	Hexachlorobenzene	118-74-1	ND	5.73	-1.31	7.04	3.74	2.29E-03	1.89E-05	
52.	Hexaconazole	79983-71-4	2.3	3.84	-6.62	10.46	3.02*	3.94E-05	6.57E-02	
53.	Hexythiazox	78587-05-0	ND	2.61	-6.06	8.67	3.79	3.03E-06	1.42E-03	
54.	Imazalil	35554-44-0	6.49	3.82	-6.74	10.56	3.73	3.21E-04	7.11E-01	
55.	Imidacloprid	138261-41-3	ND	0.57	-12.66	13.23	3.14*	8.05E-10	1.49E+00	
56.	Indoxacarb	173584-44-6	ND	4.65	-7.57	12.22	3.65	2.53E-08	3.79E-04	
57.	Iprodione	36734-19-7	ND	3.00	-7.98	10.98	2.85	1.10E-06	4.21E-02	
58.	Isoproturon	34123-59-6	ND	2.87	-8.38	11.25	2.89*	3.29E-06	3.15E-01	
59.	Lambda-Cyhalothrin	91465-08-6	ND	7.00	-4.80	11.80	5.26	4.33E-07	1.11E-05	
60.	Lindane (gamma-hexachlorocyclohexane	58-89-9	ND	4.14	-3.96	8.10	3.04	7.53E-03	2.75E-02	
61.	Linuron	330-55-2	ND	3.20	-6.59	9.79	2.7	1.91E-04	3.01E-01	
62.	Malathion	121-75-5	ND	2.36	-6.45	8.81	2.36	4.51E-04	5.14E-01	
63.	Mancozeb	8018-01-7	10.3	2.24	-5.83	8.07	3.00	9.62E-05	2.62E-02	
64.	Maneb	12427-38-2	ND	-0.51	-7.90	7.39	3.30	2.41E-05	7.70E-01	5.28E-03
65.	Mefenoxam (Metalaxyl-M)	70630-17-0	ND	1.71	-7.55	9.26	1.57	6.45E-03	9.31E+01	
66.	Metalaxyl	57837-19-1	ND	1.71	-7.41	9.12	1.57	3.31E-03	3.45E+01	
67.	Metaldehyde	108-62-3	ND	0.22	-2.68	2.90	2.38	6.60E+00	1.26E+00	
68.	Methiocarb	2032-65-7	ND	2.92	-7.01	9.93	2.32	2.89E-05	1.20E-01	1.38E+02

69.	Methoxychlor	72-43-5	ND	5.08	-3.65	8.73	4.90	1.61E-04	2.89E-04	
70.	Metribuzin	21087-64-9	1.3	1.70	-8.03	9.73	1.71	1.12E-04	4.90E+00	
71.	Metsulfuron-methyl	74223-64-6	3.75	2.20			1.54		8.40E+00	
72.	monocrotophos	6923-22-4	ND	-0.20	-10.32	10.12	1.28	5.29E-04	4.48E+03	
73.	Nicosulfuron	111991-09-4	4.78	0.01	-9.50	9.51	1.4	1.40E-05	1.78E+01	
74.	Novaluron	116714-46-6	ND	5.27	-3.86	9.13	3.98	3.67E-05	1.08E-04	
75.	o,p'-DDT	789-02-6	ND		-3.52		5.18	1.80E-04	2.40E-04	
76.	Oxadiazon	19666-30-9	ND	4.80	-5.34	10.14	3.51	2.30E-05	2.03E-03	
77.	Oxamyl	23135-22-0	-2.11	-0.47	-8.01	7.54	1.00	3.07E-02	1.28E+03	
78.	p,p'-DDD	72-54-8	ND	6.02	-3.59	9.61	4.70	1.80E-04	2.81E-04	
79.	p,p'-DDE	72-55-9	ND	6.51	-2.59	9.10	4.82	8.00E-04	1.27E-04	
80.	Paraquat	4685-14-7	ND	-4.22	-11.77	7.55	6	1.40E-05	3.33E+03	
81.	Penconazole	66246-88-6	1.51	3.66	-6.24	9.90	4.08*	3.71E-04	2.57E-01	
82.	Pendimethalin	40487-42-1	2.8	5.20	-3.17	8.37	3.7	1.95E-03	1.17E-03	2.35E+02
83.	Pirimicarb	23103-98-2	4.4	1.70	-7.46	9.16	1.90	9.71E-04	1.13E+01	
84.	Pirimiphos-methyl	29232-93-7	4.3	4.20	-4.43	8.63	3.00	3.82E-03	4.13E-02	
85.	Prochloraz	67747-09-5	3.8	4.10	-6.17	10.27	3.25	1.51E-04	9.03E-02	
86.	Propanil	709-98-8	19.1	3.07	-7.15	10.22	2.17	1.21E-04	6.97E-01	
87.	Propazine	139-40-2	1.7	2.93	-6.73	9.66	2.40	1.75E-05	3.74E-02	
88.	Propiconazole	60207-90-1	1.09	3.72	-7.15	10.87	3.39	5.60E-05	3.21E-01	
89.	Propoxur	114-26-1	ND	1.52	-6.90	8.42	1.67	2.80E-03	8.89E+00	
90.	Pyraclostrobin	175013-18-0	ND	3.99	-8.34	12.33	3.97	6.36E-08	5.62E-03	6.24E+01
91.	Pyrimethanil	53112-28-0	3.52	2.84	-5.84	8.68	3.1*	2.20E-03	6.07E-01	
92.	Simazine	122-34-9	1.62	2.18	-7.41	9.59	2.10	2.95E-06	3.07E-02	
93.	Spiroxamine	118134-30-8	6.9	2.83	-5.36	8.19	4.88*	1.71E-02	1.58E+00	
94.	Tebuconazole	107534-96-3	5	3.70	-7.95	11.65	3.53*	3.78E-06	1.34E-01	3.12E+02
95.	Tebufenozide	112410-23-8	ND	4.25	-6.29	10.54	2.74*	3.00E-06	2.35E-03	
96.	Tebuthiuron	34014-18-1	ND	1.79	-8.83	10.62	1.83	4.00E-05	1.10E+01	
97.	Terbuthylazine	5915-41-3	1.9	3.40	-6.03	9.43	2.32	9.00E-05	3.92E-02	5.22E+01
98.	Terbutryn	886-50-0	4.3	3.74	-6.06	9.80	2.85	2.25E-04	1.04E-01	5.39E+02
99.	Thiabendazole	148-79-8	4.73	2.47	-9.06	11.53	3.24	5.33E-07	2.48E-01	
100.	Thiacloprid	111988-49-9	ND	1.20	-12.47	13.67	3.29*	6.18E-10	7.32E-01	

101.	Thiamethoxam	153719-23-4	ND	-0.13	-12.72	12.59	1.75	6.60E-09	1.41E+01	
102.	Thifensulfuron	79277-67-1	ND				1.9*			
103.	Thiophanate-methyl	23564-05-8	7.28	1.40	-7.31	8.71	3.25	9.51E-06	7.77E-02	
104.	Thiram	137-26-8	8.19	1.73	-5.13	6.86	2.83	2.29E-03	1.25E-01	
105.	Triadimenol	55219-65-3	ND	3.08	-8.72	11.80	2.7	1.32E-06	2.79E-01	
106.	Triazophos	24017-47-8	ND	3.34	-6.19	9.53	2.55	1.97E-04	1.24E-01	
107.	Triclopyr	55335-06-3	3.97	-0.51	-7.40	6.89	1.67	1.68E-04	1.72E+00	
108.	Trifloxystrobin	141517-21-7	ND	4.50	-6.04	10.54	3.52*	3.40E-06	1.49E-03	
109.	α-Endosulfan	959-98-8	ND	4.68	-3.16	7.84	4.06	1.57E-03	9.03E-04	
110.	β-Endosulfan	33213-65-9	ND	3.77					1.27E-03	

Table S2: Pesticides categories based on the reliability and overall availability of physicochemical properties data

S/N	Active ingredient	Difference between Consensus Predicted Values (CPVs) and Final Adjusted Values (FAVs)					
		Log K_{AW}	Log K_{OA}	Log K_{OW}	Log K_{OC}	WS (mol/m^3)	VP (Pa)
CATEGORY 1 (High data availability; high data reliability) – 27 % of pesticides							
1	Alachlor	0.09	0.00	0.13	0.04	0.431	0.210
2	Ametryn	0.08	0.39	0.09	0.14	0.009	0.608
3	Bentazon	0.74	0.30	0.44	0.28	0.319	0.443
4	Butachlor	0.03	0.34	0.12	0.19	0.336	0.130
5	Cadusafos	0.19	0.18	0.20	0.03	0.36	0.46
6	Carbofuran	0.14	0.05	0.20	0.11	0.006	0.845
7	DDT (p,p'-DDT)	0.03	0.22	0.10	0.08	0.978	0.377
8	Diazinon	0.30	0.58	0.20	0.11	0.618	0.041
9	Dimethoate	0.20	0.57	0.05	0.33	0.048	0.013
10	Endrin	0.78	0.00	0.14	0.35	0.594	0.702
11	Ethoprophos	0.14	0.07	0.42	0.13	0.469	0.137
12	Fenamiphos	0.33	0.39	0.08	0.04	0.465	0.079
13	Heptachlor	0.25	0.38	0.46	0.20	0.592	0.736
14	Imazalil	0.54	0.38	0.32	0.10	0.272	0.317
15	Linuron	0.03	0.07	0.07	0.18	0.255	0.665
16	Malathion	0.50	0.38	0.25	0.56	0.031	0.665

17	Mefenoxam (Metalaxyl-M)	0.52	0.30	0.05	0.26	0.260	0.95
18	Metalaxyl	0.52	0.30	0.05	0.26	0.260	0.95
19	Oxadiazon	0.06	0.47	0.00	0.11	0.459	0.04
20	Oxamyl	0.42	0.85	0.17	0.00	0.427	0.76
21	p,p'-DDD	0.58	0.20	0.22	0.21	0.964	0.319
22	p,p'-DDE	0.04	0.07	0.14	0.43	0.768	0.090
23	Pirimicarb	0.43	0.27	0.07	0.32	0.147	0.590
24	Propiconazole	0.19	0.32	0.18	0.09	0.405	0.51
25	Propoxur	0.14	0.40	0.28	0.05	0.158	0.60
26	Pyrimethanil	0.92	0.86	0.07	0.58	0.43	0.69
27	Tebuconazole	0.07	0.51	0.07	0.63	0.13	0.31
28	Tebuthiuron	0.45	0.12	0.13	0.37	0.369	0.335
29	Terbutryn	0.27	0.34	0.08	0.09	0.221	0.548
30	Triadimenol	0.70	1.00	0.07	0.24	0.297	0.370
CATEGORY 2 (High data availability; low reliability for some data) – 69 % of pesticides							
1	Abamectin	3.41	1.92	1.94	1.44	2.46	14.44
2	Hexythiazox	0.45	5.11	5.65	0.45	0.543	1.38
3	monocrotophos	0.34	0.62	0.40	0.90	1.021	0.31
4	Methiocarb	0.14	0.23	0.33	0.06	0.749	1.36
5	Triazophos	1.10	0.33	0.34	0.24	0.507	0.37
6	Dimethomorph	2.24	0.27	0.34	0.40	0.04	1.04
7	Azoxystrobin	0.03	1.18	0.09	0.25	1.327	1.31
8	Epoxiconazole	0.66	0.95	0.06	0.46	0.55	1.54
9	Thiabendazole	2.29	0.73	0.11	0.19	0.883	0.57

10	Carbendazim	0.52	1.15	0.04	0.37	1.751	1.19
11	Bitertanol	1.17	2.09	0.05	0.65	0.59	2.87
12	Benalaxyl	1.54	1.38	0.55	0.25	0.246	1.12
13	Difenoconazole	2.57	1.04	0.01	0.84	0.21	0.08
14	Mancozeb	2.45	1.50	1.16	0.25	5.476	0.04
15	Iprodione	1.86	0.19	0.68	0.56	0.811	1.00
16	Prochloraz	1.68	0.78	0.86	0.75	0.294	1.68
17	Maneb	0.56	0.34	0.76	0.55	3.540	1.11
18	Fenpropimorph	0.92	0.05	0.19	0.19	0.57	1.11
19	Chlorothalonil	0.34	0.30	0.40	0.20	1.231	0.68
20	Hexachlorobenzene	0.21	0.13	0.04	0.36	0.514	1.05
21	Captan	0.11	0.26	0.65	0.57	1.762	0.16
22	Boscalid	1.13	0.84	1.27	0.32	0.40	0.95
23	Spiroxamine	0.09	5.43	5.06	1.57	1.29	0.48
24	Pyraclostrobin	2.46	0.32	0.68	0.15	0.526	0.88
25	Trifloxystrobin	0.56	0.49	1.29	1.60	0.14	1.60
26	Thiophanate-methyl	1.89	0.36	0.23	0.90	1.639	0.76
27	Fenbuconazole	2.70	0.81	0.66	0.04	1.23	1.03
28	Hexaconazole	0.71	0.09	0.04	0.11	0.03	1.01
29	Penconazole	1.11	4.41	5.01	0.80	0.67	0.19
30	Cymoxanil	0.01	0.14	1.35	0.47	1.410	0.06
31	Thiram	1.21	0.26	0.01	0.56	1.445	0.55
32	Propanil	0.65	0.58	0.01	0.11	0.128	1.03
33	2,4-Dichlorophenoxyacetic acid	2.59	2.60	0.23	0.09	0.435	1.65

34	Diuron	0.02	0.19	0.11	0.21	0.771	1.12
35	Paraquat	2.62	2.65	4.50	3.82	1.004	3.53
36	Clethodim	1.36	4.96	7.08	1.65	2.13	1.26
37	Pendimethalin	1.18	0.91	0.21	0.00	0.458	0.25
38	Terbuthylazine	0.24	0.51	0.24	0.01	0.787	1.07
39	Chlorotoluron	0.27	0.34	0.12	0.08	0.682	1.34
40	Glyphosate	2.55	1.26	2.21	1.49	0.944	0.59
41	Triclopyr	0.85	2.51	4.77	0.03	0.539	0.63
42	Nicosulfuron	5.04	4.89	0.33	0.66	1.110	5.67
43	Atrazine	0.15	0.61	0.15	0.22	1.033	1.34
44	Cyanazine	1.15	1.57	0.21	0.44	0.659	2.49
45	Metribuzin	0.93	1.17	0.03	0.27	0.599	0.45
46	Propazine	0.14	0.62	0.06	0.16	1.116	1.28
47	Simazine	0.16	0.62	0.17	0.31	1.814	2.05
48	Isoproturon	0.02	0.72	0.20	0.85	0.66	1.18
49	Chlorpyrifos	0.19	1.01	0.08	0.01	0.150	0.222
50	Novaluron	5.88	3.88	0.29	0.08	0.344	2.34
51	Carbaryl (1-naphthyl N-methylcarbamate)	0.00	0.05	0.09	0.15	0.741	1.04
52	Fenoxycarb	0.67	0.60	0.11	0.42	0.009	1.33
53	Tebufenozide	1.72	0.05	0.98	0.85	0.07	1.76
54	Thiacloprid	5.20	2.17	0.63	0.90	0.63	4.98
55	Thiamethoxam	3.16	2.61	0.56	0.50	0.842	4.28
56	Acetamiprid	4.53	4.11	1.20	0.22	0.290	3.67
57	Imidacloprid	3.37	2.44	0.03	1.45	1.64	5.37

58	Aldrin	0.03	0.28	0.01	0.12	1.378	1.16
59	Dieldrin	0.71	0.00	0.18	0.12	1.247	1.29
60	Methoxychlor	0.49	0.15	0.24	0.38	0.293	1.13
61	o,p'-DDT	0.37	5.39	5.63	0.12	0.28	0.16
62	Endosulfan	1.39	0.81	0.55	0.12	0.970	0.80
63	beta-Hexachlorocyclohexane (β-HCH)	1.90	0.20	0.23	0.10	1.470	0.24
64	α-Endosulfan	0.30	0.57	0.43	0.22	0.184	1.35
65	Lindane (gamma-hexachlorocyclohexane	1.03	0.02	0.24	0.09	0.734	0.373
66	Indoxacarb	1.08	1.05	0.43	0.12	0.264	4.16
67	Fipronil	4.12	0.46	0.29	0.13	0.98	1.00
68	Pirimiphos-methyl	0.11	1.09	0.19	0.30	0.138	0.063
69	Cypermethrin	0.23	0.12	0.33	0.11	1.018	0.87
70	Cyphenothrin	2.23	2.34	0.41	1.14	0.035	1.71
71	Deltamethrin	0.02	0.90	0.40	1.76	0.135	0.80
72	Lambda-Cyhalothrin	0.31	0.08	0.06	0.14	0.057	1.02
73	Emamectin-benzoate	3.31	3.40	6.11	1.35	0.901	13.67
74	Bifenthrin	0.59	1.69	1.07	0.20	0.209	0.92
75	Metaldehyde	1.99	0.71	0.22	1.78	1.965	0.24
76	Brodifacoum	0.93	1.49	0.64	2.59	0.353	5.85
CATEGORY 4 (Partial data; low data reliability) – 3.6 % of pesticides							
1	Glufosinate	11.08	1.75	3.45	0.97		2.04
2	Thifensulfuron				0.52		
3	Metsulfuron-methyl	12.95	3.29	0.56	0.32	0.35	
4	β-Endosulfan	1.47	1.92	0.40		1.29	2.04

Table S3: Complete QSAR predictions showing predictions "(x)" that were excluded from CPV calculations

("(x)" following numbers are flagged because they either (1) do not meet our diagnostic inclusion criteria (molar mass > thresholds; 4 or more of the Abraham solute as "structural outliers"), (2) exceed the plausible theoretical upper limit values (19.3 for log K_{OW}, 22.3 for log K_{OA}, 16.6 for log K_{AW}, 5.0 for log Vp, and 1.4 for log Sw – see Table 1 of Brown et al. 2025[3]), or (3) are PPLFER logK_{OC} predictions for chemicals predominantly ionized at a neutral pH (i.e., the neutral fraction <50%) (PPLFER is not suited for ionized chemicals).

	MW (g/mol)	logKOW				logKOA				logKOC			logKAW				pKa		Species distribution		
Name	OPERA	OPERA	IFS-QSAR	EPI Suite	PPLFER	OPERA	IFS-QSAR	EPI Suite	PPLFER	OPERA	EPI Suite	PPLFER	OPERA	IFS-QSAR	EPI Suite	PPLFER	pKa,a_OPERA	pKa,b_OPERA	Neutral%	Cation%	Anion%
Abamectin	1732	4.70	6.78 (x)	4.39 (x)	7.97	9.62	42.5 (x)	11.6 (x)	42.2 (x)	4.94	5.94(x)	2.85(x)	-3.73	-35.2 (x)	-25.3 (x)	-36.4	7.16		37%	0%	63%
Hexythiazox	353	3.35	6.66	5.57	6.81	10.3	14.1	11.6	14.0	3.79	3.33	5.60	-5.67	-7.34	-7.03	-7.55	8.57		94%	0%	6%
monocrotophos	223	-0.20	0.60	-0.31	0.69	8.58	8.30	10.4	8.43	0.01	1.24	-0.10	-10.6	-8.24	-10.7	-8.48		6.89	76%	24 %	0%
Methiocarb	225	2.92	2.23	2.87	2.33	9.54	9.69	10.2	9.66	2.32	2.43	1.48(x)	-7.31	-7.74	-7.33	-7.92	6.65		15%	0%	85%
Triazophos	313	3.34	2.73 (x)	3.37	2.30	10.1	11.9 (x)	9.24	10.7	2.21	3.27	1.47	-5.70	-9.58 (x)	-8.50	-9.20		1.95	100 %	0%	0%
Dimethomorph	388	2.68	3.86 (x)	2.36	4.02	11.7	15.3 (x)	11.2	15.1	3.41	3.76	3.05(x)	-8.08	-11.8 (x)	-13.4	-12.1		8.27	12%	88 %	0%
Mefenoxam (Metalaxyl-M)	279	1.65	1.76	1.70	1.94	9.84	10.9	8.63	10.8	1.57	1.59	0.78	-8.02	-9.49	-7.48	-9.72		3.57	100 %	0%	0%
Metalaxyl	279	1.65	1.76	1.70	1.94	9.84	10.9	8.63	10.8	1.57	1.59	0.78	-8.02	-9.49	-7.48	-9.72		3.57	100 %	0%	0%
Pyrimethanil	199	2.84	2.71	3.19	2.90	10.4	8.41	8.68	8.31	2.87	2.73	1.97	-5.84	-5.71	-4.00	-5.86		5.09	100 %	0%	0%
Azoxystrobin	403	2.50	2.58	1.58	2.98	11.7	16.4	14.0	16.2	3.74	3.45	1.88	-11.5	-14.1	-11.5	-14.5		1.24	100 %	0%	0%
Epoxiconazole	330	3.44	3.92 (x)	3.47	3.22	10.2	13.1 (x)	11.2	11.1	2.48	4.36	2.33	-7.32	-9.34 (x)	-7.79	-8.55		2.88	100 %	0%	0%
Thiabendazole	201	2.47	2.46	2.00	2.52	10.1	10.5	11.5	10.4	3.24	3.62	2.28	-4.45	-8.29	-9.09	-8.39		5.00	100 %	0%	0%

[3] Brown, T. N., Sangion, A., Li, L., & Arnot, J. A. (2025). Quantifying uncertainty in predicted chemical partition ratios required for chemical assessments. *Environmental Science: Processes & Impacts*, *27*(11), 3457–3470. https://doi.org/10.1039/D5EM00357A

Carbendazim	191	1.52	1.35	1.55	1.48	8.41	10.3	10.6	10.2	2.35	2.58	1.02	-9.13	-9.17	-10.2	-9.30	9.94	1.26	100 %	0%	0%
Bitertanol	337	4.16	4.14	4.07	4.45	10.7	13.8	15.1	13.7	2.90	3.63	3.14	-9.13	-9.71	-10.2	-10.0	11.7		100 %	0%	0%
Benalaxyl	325	3.40	4.38	3.69	4.31	11.5	11.0	8.72	10.8	3.54	3.51	2.84	-6.24	-7.00	-7.50	-7.14		2.53	100 %	0%	0%
Difenoconazole	406	4.30	4.28 (x)	5.20	3.37	11.7	16.2 (x)	13.7	13.8	3.60	3.77	2.55	-4.59	-12.3 (x)	-9.16	-11.4	8.49	3.56	92%	0%	8%
Mancozeb	271	0.53	-0.78 (x)	0.62	-0.65	7.94	10.7 (x)	8.03	10.5	2.71	2.78	-0.48 (x)	-7.60	-12.1 (x)		-12.3	1.93		0%	0%	100 %
Iprodione	330	3.00	4.38	2.85	4.48	10.3	13.3	9.89	13.2	2.85	1.72	3.83(x)	-6.90	-9.08	-11.4	-9.25	5.88	1.95	3%	0%	97%
Prochloraz	377	4.10	2.44	4.13	2.28	11.8	13.6	10.3	12.9	2.70	3.38	1.40	-6.18	-11.7	-9.51	-11.6		3.63	100 %	0%	0%
Imazalil	297	3.82	2.99	4.10	3.10	9.84	10.9	10.8	10.8	3.73	3.93	2.22(x)	-7.16	-8.18	-5.53	-8.35		8.12	16%	84 %	0%
Maneb	265	0.79	-0.78 (x)	0.62	-0.65	7.94	10.7 (x)	8.03	10.5	2.71	2.78	-0.48 (x)	-7.60	-12.1 (x)		-12.3	1.93		0%	0%	100 %
Fenpropimorph	303	4.93	4.17	5.50	4.37	8.85	10.3	8.93	10.1	3.20	4.43	2.14	-4.59	-6.06	-5.06	-6.31		7.08	68%	32 %	0%
Chlorothalonil	266	2.98	3.36	3.66	3.18	8.49	8.03	7.89	8.26	3.26	3.02	2.92	-4.09	-4.98	-5.21	-5.46			100 %	0%	0%
Hexachlorobenzene	285	5.73	5.56	5.86	5.62	7.37	7.05	7.36	7.00	3.74	3.79	4.78	-1.16	-1.26	-1.44	-1.31			100 %	0%	0%
Captan	301	2.80	1.07 (x)	2.74	0.91	8.83	10.3 (x)	9.34	9.77	2.30	2.40	0.50	-6.57	-9.83 (x)	-6.73	-9.74		2.07	100 %	0%	0%
Boscalid	343	2.96	4.90	4.00	5.06	10.3	14.5	12.7	14.3	3.19	3.98	4.09	-7.90	-9.61	-9.76	-9.84		2.03	100 %	0%	0%
Spiroxamine	298	2.43	4.74 (x)	5.51	4.69	8.97	10.1 (x)	10.9	9.88	3.24	3.37	2.91(x)	-5.81	-5.55 (x)	-5.10	-5.69		8.97	3%	97 %	0%
Pyraclostrobin	388	3.99	4.24 (x)	5.45	4.57	11.7	15.3 (x)	12.7	15.2	3.21	4.68	3.55	-8.67	-11.1 (x)	-13.3	-11.5		5.39	99%	1%	0%
Trifloxystrobin	408	4.50	6.13 (x)	6.62	6.24	9.58	12.4 (x)	10.5	12.3	4.52	6.48	4.34	-7.82	-6.06 (x)	-5.36	-6.49		5.50	99%	1%	0%
Thiophanate-methyl	342	1.40	2.00 (x)	1.10	2.39	9.42	13.1 (x)	8.71	13.0	3.25	2.52	1.30	-7.49	-11.2 (x)	-10.9	-11.5	9.34		99%	0%	1%
Fenbuconazole	337	3.23	4.24	4.23	3.84	10.1	13.5	8.70	12.6	2.95	4.84	3.05	-7.91	-9.74	-8.21	-9.49		0.06	100 %	0%	0%
Propiconazole	342	3.72	3.83	4.13	3.91	10.2	13.2	10.9	13.1	3.39	3.19	3.32	-7.43	-9.74	-7.26	-9.93		3.33	100 %	0%	0%
Triadimenol	296	2.90	3.30	2.95	3.44	10.2	12.3	13.4	12.1	2.70	2.29	2.39	-8.85	-9.13	-9.19	-9.33	10.2		100 %	0%	0%
Tebuconazole	308	3.70	3.69	3.89	3.81	10.7	13.1	11.9	12.5	3.00	3.19	2.50	-8.40	-9.68	-7.68	-9.42	11.5	4.89	100 %	0%	0%
Hexaconazole	314	3.90	4.05	3.66	4.16	10.7	13.1	10.8	13.0	2.52	3.06	3.16	-6.88	-9.24	-8.05	-9.43	8.46		92%	0%	8%
Penconazole	284	3.71	4.27	4.67	3.87	8.62	10.5	10.9	9.45	2.96	3.93	2.96	-6.52	-6.41	-3.74	-6.05		1.85	100	0%	0%

																			%		
Cymoxanil	198	0.59	0.05 (x)	4.24	0.99	8.18	8.76 (x)	8.46	9.02	2.09	1.15	0.37(x)	-7.84	-9.03 (x)	-7.87	-8.65	6.61	2.92	14%	0%	86%
Thiram	240	1.73	2.54 (x)	1.70	1.72	7.37	10.8 (x)	6.86	8.66	2.83	2.79	1.19	-4.88	-8.52 (x)	-2.96	-7.62		6.87	77%	23 %	0%
Butachlor	312	4.50	4.55	4.84	4.59	10.8	10.8	10.2	10.6	2.86	3.28	3.01	-5.71	-6.40	-5.67	-6.57		3.07	100 %	0%	0%
Propanil	218	3.07	3.16	2.88	3.14	9.10	9.18	10.2	9.06	2.17	2.25	2.44	-6.29	-6.19	-6.74	-6.26	10.1		100 %	0%	0%
2,4-Dichlorophenoxyacetic acid	221	2.81	2.47	2.62	2.43	8.65	10.2	9.23	10.0	1.66	1.47	1.68(x)	-5.86	-7.90	-6.43	-7.96	2.42		0%	0%	100 %
Diuron	233	2.68	2.91	2.67	2.89	9.96	10.6	10.4	10.5	2.40	2.04	2.15	-7.68	-7.93	-7.66	-8.01	10.7		100 %	0%	0%
Bentazon	240	2.34	3.53	1.67	3.59	9.81	9.70	9.39	9.59	1.53	1.00	2.87	-7.30	-6.27	-8.09	-6.37	7.67		65%	0%	35%
Paraquat	186	1.07		-0.56	0.34	7.43		6.66	-0.21	3.03	3.50	0.02	-11.7		-10.9	0.59		3.27	100 %	0%	0%
Alachlor	270	3.52	3.14	3.37	3.51	9.72	9.12	9.99	9.11	2.28	2.49	2.18	-6.47	-6.32	-6.04	-6.13		3.07	100 %	0%	0%
Clethodim	360	4.34	4.10	4.21	4.35	10.6	14.3	13.5	14.1	3.46	3.90	2.76	-7.80	-10.3	-9.33	-10.6		-2.37	100 %	0%	0%
Pendimethalin	281	5.20	4.96	4.82	4.96	10.2	9.96	8.37	9.82	3.70	3.75	3.66	-4.47	-5.06	-4.23	-5.17		3.04	100 %	0%	0%
Terbuthylazine	230	3.21	3.04	3.27	3.12	8.42	9.14	9.43	9.02	2.32	2.50	2.17	-5.92	-6.24	-6.62	-6.36		4.34	100 %	0%	0%
Ametryn	227	2.98	2.93	3.32	3.06	9.07	9.82	9.98	9.69	2.59	2.63	2.12	-7.15	-7.00	-6.55	-7.15		5.27	99%	1%	0%
Glufosinate	181	1.85	-3.96 (x)	-4.49	-4.07	8.32	13.3 (x)	9.18	13.1	2.63	1.00	-4.25(x)	-8.46	-18.4 (x)	-13.7	-18.6	-0.74	10.5	0%	0%	100 %
Oxadiazon	345	4.80	4.64 (x)	4.81	4.79	9.30	12.0 (x)	10.3	11.9	3.51	3.70	3.65	-5.18	-7.45 (x)	-5.88	-7.66		4.68	100 %	0%	0%
Chlorotoluron	213	2.41	2.58	2.58	2.56	9.81	10.0	10.6	9.86	2.02	2.04	1.76	-8.23	-7.68	-7.49	-7.76	11.0		100 %	0%	0%
Linuron	249	3.20	3.17	2.91	3.24	9.93	9.62	9.79	9.51	2.70	2.53	2.33	-6.91	-6.55	-6.33	-6.66	11.9		100 %	0%	0%
Glyphosate	169	-3.39	-2.28	-4.77	-2.33	8.40	13.6	4.67	13.4	3.32	0.00	-2.70(x)	-9.65	-16.7	-16.8	-16.8	-2.68		0%	0%	100 %
Triclopyr	256	8.98	2.72	2.53	2.79	8.87	10.1	9.93	9.98	1.67	1.72	1.94(x)	-6.42	-7.45	-6.68	-7.56	2.08		0%	0%	100 %
Tebuthiuron	228	1.79	1.47	1.78	1.61	10.2	10.5	10.1	10.3	1.83	1.63	0.91	-8.30	-9.32	-9.56	-9.49	8.46		92%	0%	8%
Thifensulfuron	373	1.03	0.20 (x)	1.32	0.47	9.36	18.0 (x)	15.6	17.8	1.67	1.10	-0.03(x)	-9.73	-18.4 (x)	-14.3	-18.7	1.22		0%	0%	100 %
Metsulfuron-methyl	381	2.20	0.42 (x)	2.00	0.72	9.55	16.3 (x)	16.5	16.1	1.54	1.97	0.17	-14.4	-16.5 (x)	-11.5	-16.8		2.04	100 %	0%	0%

Nicosulfuron	410	0.01	-0.06 (x)	-1.15	0.19	9.62	18.5 (x)	16.3	18.2	1.48	1.00	-0.25	-9.99	-19.4 (x)	-16.2	-19.7		5.65	98%	2%	0%
Atrazine	216	2.61	2.16	2.82	2.26	8.38	9.07	9.58	8.94	2.24	2.35	1.46	-6.92	-7.10	-6.74	-7.23		3.79	100%	0%	0%
Cyanazine	241	2.22	1.64	2.51	1.67	9.10	10.7	12.2	10.6	2.28	2.13	1.12	-7.61	-9.55	-10.1	-9.67		1.49	100%	0%	0%
Metribuzin	214	1.70	1.75	1.49	1.97	7.51	11.1	10.0	11.0	1.71	1.73	0.88	-8.20	-9.43	-10.1	-9.62		1.08	100%	0%	0%
Propazine	230	2.93	2.60	3.24	2.71	8.41	9.39	9.66	9.26	2.40	2.54	1.80	-7.12	-6.95	-6.62	-7.09		3.93	100%	0%	0%
Terbutryn	241	3.56	3.59	3.77	3.71	9.12	9.95	9.80	9.83	2.85	2.78	2.64	-6.23	-6.42	-6.43	-6.58		5.62	98%	2%	0%
Simazine	202	2.18	1.69	2.40	1.78	8.36	8.66	9.59	8.54	2.10	2.17	1.11	-7.64	-7.21	-6.86	-7.32		3.41	100%	0%	0%
Isoproturon	206	2.68	2.57	2.84	2.57	9.80	11.1	11.2	11.0	2.00	2.30	1.82	-8.33	-8.89		-9.00	11.0		100%	0%	0%
Chlorpyrifos	351	4.96	5.24	5.11	4.86	10.6	8.96	8.88	9.83	3.70	3.86	3.49	-3.92	-3.77	-3.99	-5.34		2.03	100%	0%	0%
Novaluron	493	5.27	6.53 (x)	5.26	6.14	9.47	12.1 (x)	15.8	11.9	4.10	3.58	4.50	-9.37	-5.52 (x)	-10.6 (x)	-6.10	12.4		100%	0%	0%
Carbaryl (1-naphthyl N-methylcarbamate)	201	2.36	2.02	2.35	2.36	9.13	8.72	9.23	9.26	2.40	2.55	1.81	-6.85	-6.93	-6.89	-7.42	8.14		85%	0%	15%
Carbofuran	221	1.98	1.97	2.30	2.25	9.04	8.48	10.1	8.76	1.75	1.98	1.25(x)	-7.69	-6.81	-7.18	-7.05	6.88		23%	0%	77%
Fenoxycarb	301	4.30	4.52	4.24	4.56	10.9	12.0	12.1	11.9	3.00	3.69	3.58	-7.64	-7.72	-9.23	-7.88	8.59		94%	0%	6%
Propoxur	209	1.52	2.10	1.90	-0.57	9.22	8.68	8.42	2.40	1.67	1.78	-2.37(x)	-7.22	-6.79	-6.86	-3.50	6.81		20%	0%	80%
Oxamyl	219	-0.47	-0.49	-1.20	-0.40	9.23	9.58	7.54	9.40	1.00	1.00	-1.00(x)	-8.02	-10.6	-8.84	-10.8	5.97	3.26	4%	0%	96%
Pirimicarb	238	1.70	1.92	1.40	2.05	8.63	9.42	9.16	9.27	1.90	1.75	1.09	-7.10	-7.76	-6.97	-7.93		4.63	100%	0%	0%
Tebufenozide	352	4.25	6.34	4.62	5.70	10.4	15.1	10.5	13.4	3.28	3.49	4.00	-7.57	-8.82	-8.45	-8.28	9.81		100%	0%	0%
Thiacloprid	253	1.26	1.86	2.33	1.88	8.17	10.4	14.7	10.3	2.49	3.05	1.64	-6.40	-9.07	-8.00	-9.19		0.75	100%	0%	0%
Thiamethoxam	292	-0.13	1.01	0.80	0.04	7.38	11.2	12.6	10.4	2.08	2.42	-0.59(x)	-6.48	-10.5	-12.6	-11.4	4.37		0%	0%	100%
Acetamiprid	223	1.83	1.82	2.55	1.78	6.88	9.51	8.10	9.36	2.08	2.70	1.47	-7.00	-8.21	-5.55	-8.29		2.50	100%	0%	0%
Imidacloprid	256	0.57	0.40	0.56	0.61	8.83	9.81	13.7	9.67	2.06	2.99	0.02	-8.26	-9.77	-11.4	-9.96		1.93	100%	0%	0%
Aldrin	365	6.50	6.54	6.75	6.16	8.66	8.53	9.24	8.50	4.69	4.91	4.81	-2.27	-1.76	-1.80	-2.40			100%	0%	0%

Dieldrin	381	5.12	5.77	5.45	5.18	8.56	9.33	8.59	10.2	4.08	4.30	4.23	-3.47	-3.54	-4.66	-5.29			100 %	0%	0%
Endrin	381	5.12	5.77	5.45	3.91	8.56	9.33	8.59	8.64	4.08	4.30	2.82	-3.47	-3.54	-4.66	-5.14			100 %	0%	0%
Heptachlor	373	6.10	5.79	5.86	5.98	7.77	9.33	7.39	9.26	4.38	4.62	4.75	-1.92	-3.25	-2.14	-3.40			100 %	0%	0%
Methoxychlor	346	5.08	5.27	5.67	5.26	9.17	11.4	10.2	11.3	4.90	4.43	4.24	-5.09	-6.32	-5.40	-6.45			100 %	0%	0%
DDT (p,p'-DDT)	354	6.79	6.69	6.79	6.96	9.57	10.0	10.4	9.88	5.10	5.23	5.83	-3.47	-3.31	-3.21	-2.99			100 %	0%	0%
o,p'-DDT	354	6.91	6.42	6.79	6.53	9.57	10.2	10.3	9.50	5.31	5.24	5.34	-3.10	-3.80	-3.21	-3.08			100 %	0%	0%
p,p'-DDD	320	6.13	6.48	5.87	6.46	10.0	9.94	9.59	9.83	4.21	5.07	5.44	-3.57	-3.40	-2.75	-3.48			100 %	0%	0%
p,p'-DDE	316	6.73	6.85	6.00	7.00	9.44	9.24	9.28	9.66	4.82	5.07	5.87	-2.77	-2.20	-2.84	-2.65			100 %	0%	0%
Endosulfan	407	3.83	5.08	3.50	5.12	8.81	9.52	6.41	9.41	4.11	3.83	3.97	-3.28	-4.45	-5.43	-4.57			100 %	0%	0%
beta-Hexachlorocyclohexane (β-HCH)	288	3.72	3.90	4.26	3.75	8.09	7.96	7.82	7.63	3.17	3.45	2.79	-3.88	-3.95	-1.98	-4.16			100 %	0%	0%
α-Endosulfan	407	3.83	5.08	3.50	4.85	8.81	9.52	6.41	10.0	4.11	3.83	3.60	-3.28	-4.45		-5.56			100 %	0%	0%
β-Endosulfan	407	3.83	5.08	3.50	5.12	8.81	9.52	6.41	9.41	4.11	3.83	3.97	-3.28	-4.45		-4.57			100 %	0%	0%
Lindane (gamma-hexachlorocyclohexane	291	3.72	3.90	4.26	3.73	8.09	7.96	7.82	7.61	3.17	3.45	2.78	-3.88	-3.95	-1.98	-4.16			100 %	0%	0%
Diazinon	304	3.81	4.24	3.86	4.11	9.83	9.06	9.14	8.69	2.75	3.48	2.35	-5.33	-4.95	-5.45	-5.01		3.55	100 %	0%	0%
Dimethoate	229	0.78	0.90	0.72	0.94	9.92	9.42	8.78	9.26	1.20	1.11	0.30	-7.33	-8.95	-9.07	-9.06		2.45	100 %	0%	0%
Malathion	330	2.36	2.95	2.29	2.83	9.61	9.43	9.06	9.21	2.36	1.50	1.55	-6.70	-6.96	-7.47	-7.06			100 %	0%	0%
Ethoprophos	242	3.59	2.96	3.14	2.98	8.64	7.76	8.77	7.64	1.85	2.33	1.76	-5.18	-5.01	-4.90	-5.13			100 %	0%	0%
Indoxacarb	528	4.65	3.40 (x)	4.60	3.42	11.7	19.1 (x)	12.2	18.9	3.64	3.91	2.86(x)	-7.33	-16.3 (x)	-11.0 (x)	-16.8	6.61		14%	0%	86%
Fipronil	437	4.00	2.20	6.64	2.01	10.5	15.2	11.5	15.0	2.61	3.77	1.71(x)	-7.25	-13.6	-15.9	-14.1	7.36		48%	0%	52%
Pirimiphos-methyl	305	4.20	3.90	4.00	3.95	10.8	9.60	8.81	9.44	3.00	2.57	2.52	-5.27	-5.85	-3.99	-6.00		3.97	100 %	0%	0%
Cypermethrin	416	6.60	7.05 (x)	6.38	6.85	11.7	12.9 (x)	11.7	14.5	5.00	4.90	5.44	-4.81	-6.12 (x)	-4.49	-8.19			100 %	0%	0%
Cyphenothrin	375	6.29	7.44 (x)	6.49	7.32	11.8	12.2 (x)	10.3	12.0	4.82	4.90	5.59	-5.48	-4.88 (x)	-3.82	-5.02			100 %	0%	0%

Deltamethrin	505	6.20	7.52 (x)	6.18	7.43	11.7	14.0 (x)	9.89	13.8	4.79	4.90	6.04	-3.71	-6.63 (x)	-5.61 (x)	-6.79			100 %	0%	0%
Lambda-Cyhalothrin	450	6.80	7.30 (x)	6.85	7.18	11.7	11.9 (x)	11.2	11.9	5.26	5.53	5.41	-6.42	-4.91 (x)	-3.26	-5.13			100 %	0%	0%
Emamectin-benzoate	2003	1.87	7.59 (x)	5.38 (x)	8.81	9.62	42.1 (x)	12.2 (x)	41.8 (x)	4.94	6.46(x)	3.51	-3.68	-33.9 (x)		-35.1	7.47		54%	0%	46%
Bifenthrin	423	6.00	7.16	8.15	6.98	10.5	11.3	12.5	11.1	5.35	6.36	4.94	-3.34	-4.17	-3.11	-4.48			100 %	0%	0%
Cadusafos	270	3.90	3.22 (x)	3.98	3.22	8.53	8.62 (x)	8.18	8.44	2.60	2.74	1.76	-4.28	-5.63 (x)	-4.65	-5.76			100 %	0%	0%
Metaldehyde	176	0.12	-0.59	0.85	-0.36	4.31	5.74	2.89	5.59	2.38	1.00	-1.58	-2.77	-6.52	-6.54	-6.68			100 %	0%	0%
Fenamiphos	303	3.23	3.00	3.29	3.10	11.2	11.1	10.7	11.0	2.51	2.60	1.75(x)	-6.92	-8.39	-8.40	-8.58	6.33		8%	0%	92%
Brodifacoum	523	6.16	8.71	7.62	8.97	11.7	20.3	19.2	20.2	5.08	6.89	7.69	-6.39	-11.5	-10.7 (x)	-11.9			100 %	0%	0%

Table S4: Predicted exposure indices, Drinking Water Exposure Potential (DWEP) and intake fractions (*i*Fs), based on four scenarios representing predicted and empirical pesticide partitioning and reactivity data

	DWEP				*i*F			
Pesticide Active Ingredient	**Scenario 1**	**Scenario 2**	**Scenario 3**	**Scenario 4**	**Scenario 1**	**Scenario 2**	**Scenario 3**	**Scenario 4**
2,4-Dichlorophenoxyacetic acid	5.71E-12	1.24E-12	6.16E-12	1.19E-12	5.75E-15	1.25E-15	6.19E-15	1.20E-15
Acetamiprid	8.49E-11	5.61E-13	3.80E-11	4.82E-13	8.54E-14	5.65E-16	3.82E-14	4.85E-16
Alachlor	3.29E-11	1.19E-11	3.88E-11	4.76E-11	3.31E-14	1.20E-14	3.90E-14	4.79E-14
Ametryn	4.58E-11	4.56E-11	5.06E-11	6.91E-11	4.61E-14	4.59E-14	5.09E-14	6.95E-14
Atrazine	1.99E-10	8.98E-11	2.28E-10	7.12E-11	2.01E-13	9.03E-14	2.29E-13	7.17E-14
Azoxystrobin	8.53E-12	2.89E-11	8.64E-12	2.88E-11	8.58E-15	2.90E-14	8.69E-15	2.90E-14
Benalaxyl	5.25E-12	4.36E-11	5.15E-12	3.34E-11	5.28E-15	4.38E-14	5.18E-15	3.36E-14
Bentazon	2.02E-11	1.74E-11	1.80E-11	3.11E-11	2.03E-14	1.75E-14	1.81E-14	3.13E-14
Bifenthrin	9.42E-12	3.74E-12	1.15E-11	1.53E-11	9.48E-15	3.76E-15	1.15E-14	1.54E-14
Captan	1.91E-10	1.47E-13	4.39E-11	1.63E-13	1.92E-13	1.48E-16	4.42E-14	1.64E-16
Carbaryl	3.06E-11	1.48E-11	4.12E-11	9.50E-12	3.07E-14	1.48E-14	4.14E-14	9.55E-15
Chlorothalonil	9.34E-10	7.03E-12	9.25E-10	7.22E-12	9.40E-13	7.07E-15	9.31E-13	7.26E-15
Cyanazine	7.58E-11	6.87E-12	6.98E-11	5.93E-12	7.63E-14	6.91E-15	7.03E-14	5.96E-15
Cypermethrin	1.44E-11	2.53E-12	1.49E-11	7.01E-12	1.44E-14	2.54E-15	1.49E-14	7.06E-15
Deltamethrin	2.32E-12	1.91E-12	2.46E-12	2.97E-12	2.33E-15	1.92E-15	2.47E-15	2.98E-15
Diazinon	4.08E-12	1.31E-12	3.98E-12	2.07E-12	4.10E-15	1.32E-15	4.01E-15	2.09E-15
Dieldrin	9.17E-10	2.87E-10	3.34E-10	6.02E-13	9.22E-13	2.88E-13	3.36E-13	6.05E-16
Diuron	4.41E-11	1.63E-10	3.76E-11	5.93E-11	4.43E-14	1.64E-13	3.78E-14	5.96E-14
Endosulfan	7.76E-10	9.13E-11	6.79E-10	3.58E-11	7.81E-13	9.18E-14	6.83E-13	3.60E-14
Ethoprophos	1.30E-11	8.78E-12	1.51E-11	1.38E-11	1.31E-14	8.83E-15	1.52E-14	1.39E-14
Fenamiphos	1.19E-11	2.01E-13	1.19E-11	2.33E-13	1.20E-14	2.03E-16	1.20E-14	2.34E-16
Glyphosate	1.58E-12	7.09E-15	1.56E-12	7.57E-15	1.59E-15	7.13E-18	1.57E-15	7.61E-18
Indoxacarb	1.14E-10	3.52E-11	1.16E-10	3.54E-11	1.14E-13	3.54E-14	1.17E-13	3.56E-14

Iprodione	3.75E-11	8.43E-12	3.71E-11	8.37E-12	3.77E-14	8.48E-15	3.73E-14	8.42E-15
Lambda-Cyhalothrin	3.40E-12	4.27E-12	3.57E-12	5.41E-12	3.42E-15	4.29E-15	3.60E-15	5.44E-15
Lindane	3.17E-10	1.43E-09	4.95E-10	4.11E-10	3.19E-13	1.44E-12	4.98E-13	4.14E-13
Linuron	1.09E-10	6.72E-11	1.11E-10	5.33E-11	1.09E-13	6.76E-14	1.12E-13	5.36E-14
Malathion	1.95E-12	3.86E-14	1.76E-12	3.79E-14	1.96E-15	3.88E-17	1.77E-15	3.81E-17
Metalaxyl	6.62E-12	3.60E-12	6.07E-12	2.33E-12	6.66E-15	3.63E-15	6.11E-15	2.35E-15
Metaldehyde	1.98E-10	3.67E-12	2.04E-10	4.80E-12	1.99E-13	3.69E-15	2.06E-13	4.83E-15
Nicosulfuron	1.17E-11	6.51E-12	1.36E-11	2.78E-11	1.18E-14	6.55E-15	1.37E-14	2.79E-14
Novaluron	1.42E-10	3.63E-12	1.59E-10	7.94E-12	1.43E-13	3.65E-15	1.60E-13	7.99E-15
Oxadiazon	5.30E-11	4.44E-10	4.92E-11	3.46E-10	5.33E-14	4.46E-13	4.94E-14	3.48E-13
Oxamyl	6.05E-12	3.34E-12	5.61E-12	1.66E-12	6.08E-15	3.36E-15	5.64E-15	1.67E-15
Pendimethalin	2.24E-10	2.98E-11	2.18E-10	3.51E-11	2.25E-13	2.99E-14	2.19E-13	3.53E-14
Pirimiphos-methyl	2.34E-11	6.31E-12	1.63E-11	5.77E-12	2.35E-14	6.34E-15	1.64E-14	5.80E-15
Prochloraz	5.53E-11	1.49E-10	5.50E-11	2.51E-10	5.56E-14	1.50E-13	5.54E-14	2.52E-13
Propanil	8.36E-11	1.32E-13	9.09E-11	1.41E-13	8.41E-14	1.33E-16	9.14E-14	1.42E-16
Propoxur	6.22E-11	5.75E-11	2.72E-11	6.29E-11	6.25E-14	5.79E-14	2.73E-14	6.33E-14
Pyraclostrobin	2.42E-11	6.77E-13	2.42E-11	7.09E-13	2.44E-14	6.81E-16	2.43E-14	7.13E-16
Tebuthiuron	1.72E-11	4.20E-10	1.67E-11	1.03E-09	1.73E-14	4.22E-13	1.68E-14	1.04E-12
Terbutryn	7.14E-11	4.89E-11	7.56E-11	4.83E-11	7.18E-14	4.92E-14	7.61E-14	4.86E-14
Thiamethoxam	1.07E-11	2.78E-11	1.15E-11	2.69E-11	1.08E-14	2.79E-14	1.16E-14	2.71E-14
Triazophos	5.21E-12	2.82E-11	6.10E-12	3.62E-11	5.25E-15	2.84E-14	6.13E-15	3.64E-14
Triclopyr	1.48E-11	5.43E-12	1.55E-11	3.55E-14	1.49E-14	5.46E-15	1.56E-14	3.58E-17