Direct prediction of bioaccumulation of organic contaminants in plant roots from soils with machine learning models based on molecular structures

Supplementary Information

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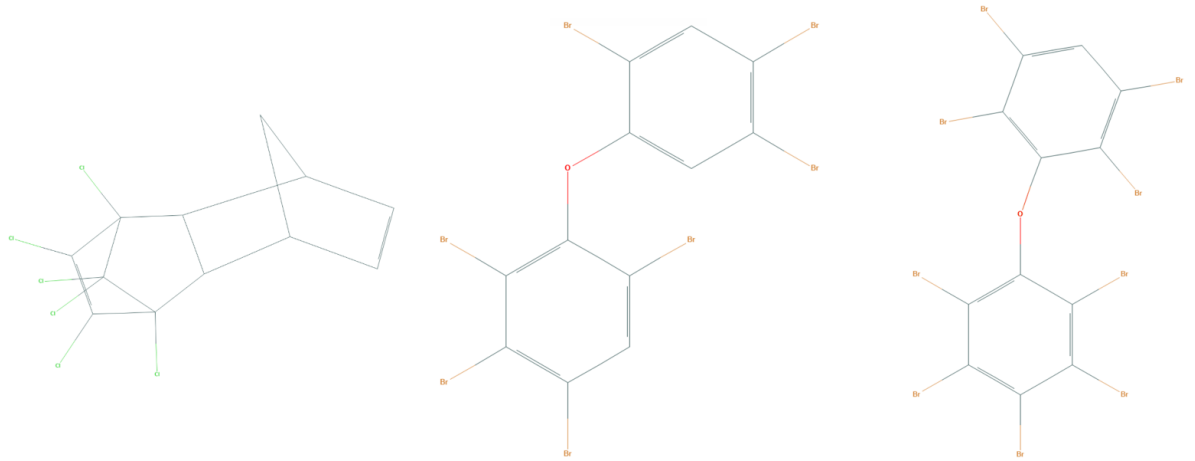
ECFP and Morgan Fingerprint: The idea behind ECFP fingerprint traces back to the Morgan algorithm, which assigns a unique, sequential atom numbering for molecules through an iterative process until every atom identifier is unique, then the intermediate atom identifiers are discarded. However, ECFP has made a few changes to the Morgan algorithm. ECFP fingerprint is defined as the set of initial atom identifiers, and all identifiers after each iteration up to the limit of n iterations. As n increases, this fingerprint set includes all identifiers found in both previous iterations and the current one. For example, ECFP fingerprint for n = 0 consists of the set of unique atom identifiers; with n = 1, it augments current set with identifiers computed by examining each atom and its immediate neighbors and assigning a new unique number; with n = 2, new identifiers for neighbors of neighbors are further included. This whole set defines the extended-connectivity fingerprint.



Aldrin

2,2',3,4,4',5',6-heptabromodiphenyl ether

2,2',3,3',4,5,5',6,6'-nonabromodiphenyl ether

Fig. S1 Chemical structures of 2,2',3,4,4',5',6-heptabromodiphenyl ether, 2,2',3,3',4,5,5',6,6'-nonabromodiphenyl ether and Aldrin

Table S1: Clustering results based on chemical structures.

Group 0 (32)	Group 1 (16)	Group 2 (15)	Group 3 (9)
Penconazole, Aldrin, Dieldrin, p-DCB (1,4-DCB), 1,2,4-TCB, alpha-HCH, HCB, o,p'-DDE, p,p'-DDE, o,p'-DDD, p,p'-DDD, o,p'-DDT, p,p'-DDT, PCB 101, PCB 153, PCB 138, PCB 180, 1,2,3,5-TeCB, Pentachlorobenzene, Arazine, Galaxolide, Tonalide, Triclocarban, Triclosan, alpha-endosulfan, Endosulfan sulfate, Heptachlor, Heptachlor epoxide, Imidacloprid, Acetamiprid, Tebuconazole, Difenoconazole	BDE-100, BDE-153, BDE-154, BDE-17 BDE-183 BDE-206, BDE-209, BDE-28, BDE-47, BDE-99, BDE-6, BDE-85, BDE-191, BDE-197, BDE-208, BDE-207	Phenanthrene, Anthracene, Fluoranthene, Benzo[a]pyrene, Pyrene, Naphthalene, Acenaphthene, Benzo[a]anthracene, Chrysene, benzo[b]fluoranthene, benzo[k]fluoranthene, Dibenzo [a,h] anthracene, Benzo [g,h,i] perylene, Benzo [e]pyrene, Indeno [1,2,3-cd] pyrene	m-DCB (1,3-DCB), o-DCB (1,2-DCB), Fluorene, Di(2-ethylhexyl) phthalate, alpha-HBCD, Trimethoprim, Carbamazepine, Tricyclazole, Azoxystrobin

Table S2: Similarity comparison of each molecular pair in the dataset (attached in a separate spreadsheet)

Gradient Boosting Regression Tree: Gradient boosting regression tree model is a prediction model that utilizes multiple weak learners to perform regression tasks. Given input features x_i and target y_i, the model calculates:

$$\widehat{y_i} = F_M(x_i) = \sum_{m=1}^{M} h_m(xi)$$

Here h_m are the weak learners, which are decision trees in this study. $\widehat{y_i}$ are the predicted values through the model.

Gradient boosting regression tree model is built in a greedy way:

$$F_M(x_i) = F_{M-1}(x_i) + h_m(x)$$

where the newly added tree $h_m(x)$ is fitted in order to minimize a sum of *loss* given the previous ensemble F_{M-1}:

$$h_m = argminL_m = argmin \sum_{i=1}^{n} loss\big(y_i, F_{M-1}(x_i) + h(x_i)\big)$$

Here $loss$ is the loss function chosen according to specific tasks. For regression tasks, a mean squared error loss function can be used. In other words, during the gradient descent procedure, a new tree that can reduce the loss is added to the model to correct or improve the final output of the model.

Impurity feature importance: The basic idea is that for individual decision trees, they perform feature selection by selecting appropriate split points. Therefore, the more often a feature is used in the split points of a tree, the more important that feature is. This notion of importance can be extended to decision tree ensembles by simply averaging the impurity-based feature importance

of each tree. However, one drawback of impurity feature importance is that it is biased towards high cardinality features.

Partial Dependence Plot: Partial dependence plot can be used to show the marginal effect of one feature have on the predicted outcome of a machine learning model. The influences of changes of $logK_{ow}$, f_{om}, f_{lipid} and MW in forms of their z-scored values on the predicted $logRCF_{soil}$ were shown in Fig. S1. For example, the predicted $logRCF_{soil}$ first remain almost unchanged when f_{lipid} is smaller than -1.2. Then $logRCF_{soil}$ decreased as z-scored value of f_{lipid} increased between -1.2 and -0.9. $logRCF_{soil}$ then increased when f_{lipid} is larger than -0.9 and decreased again when f_{lipid} $is\ larger\ than\ -0.4$. The relationship between $logRCF_{soil}$ and other corresponding property descriptor variables are even more complicated, showing much more complicated relationships than simple linearity.

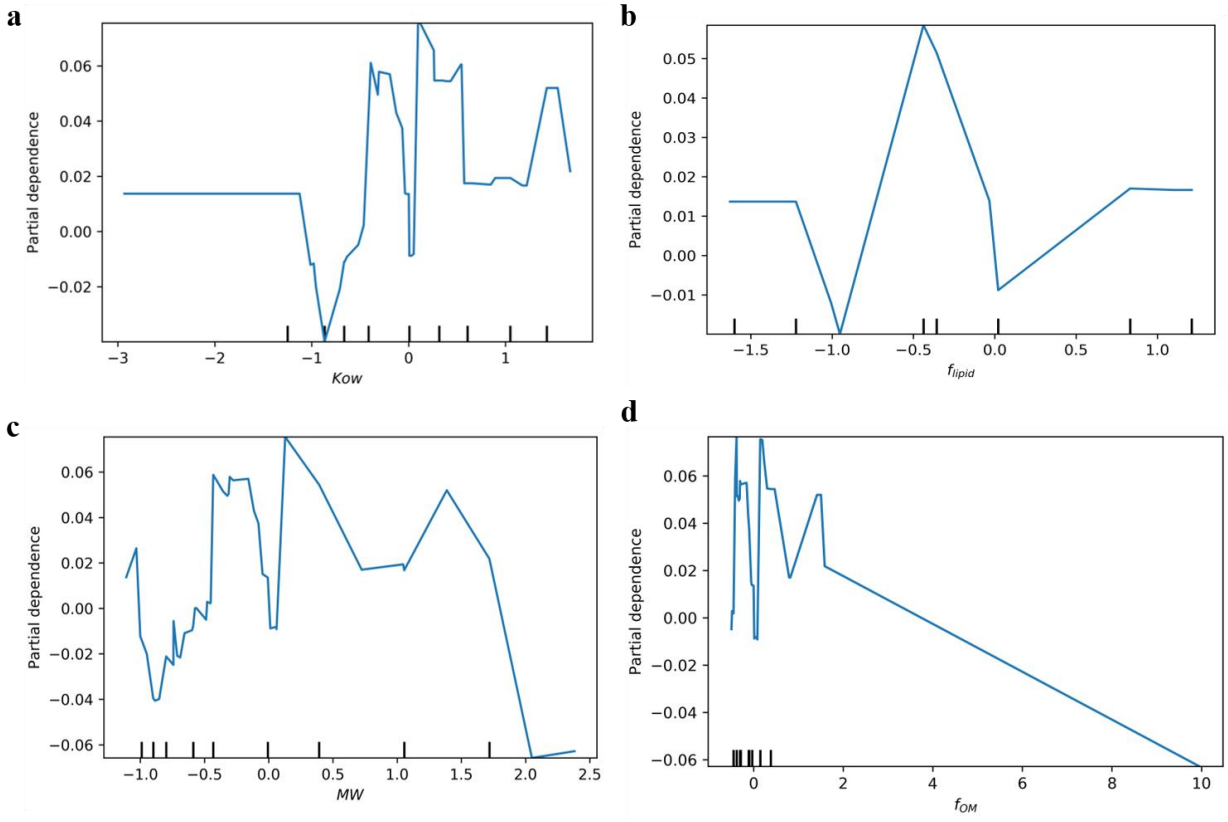


Fig. S2 Partial dependence plot of four property descriptors: (a) $logK_{ow}$; (b) f_{lipid}; (c) MW; (d) f_{om}.

Table S3: RCF_{soil} dataset

Compounds	log Kow	fom (%)	MW	SMILES	flip (%)	log RCF-water	log RCF-soil	Citation	Plant
Penconazole	3.72	0.97	284.18	CCCC(CN1C=NC=N1)C2=C(C=C(C=C2)Cl)Cl	1.10	1.57	-0.03	Jiang et al., 2016	Wheat
Penconazole	3.72	3.26	284.18	CCCC(CN1C=NC=N1)C2=C(C=C(C=C2)Cl)Cl	1.10	1.66	-0.19	Jiang et al., 2016	Wheat
Penconazole	3.72	5.03	284.18	CCCC(CN1C=NC=N1)C2=C(C=C(C=C2)Cl)Cl	1.10	1.63	-0.30	Jiang et al., 2016	Wheat
Penconazole	3.72	1.59	284.18	CCCC(CN1C=NC=N1)C2=C(C=C(C=C2)Cl)Cl	1.10	1.47	-0.13	Jiang et al., 2016	Wheat
Penconazole	3.72	2.60	284.18	CCCC(CN1C=NC=N1)C2=C(C=C(C=C2)Cl)Cl	1.10	1.46	-0.25	Jiang et al., 2016	Wheat
Aldrin	5.66	3.60	364.9	C1C2C=CC1C3C2C4(C(=C(C3(C4(Cl)Cl)Cl)Cl)Cl)Cl	0.24	1.63	-1.38	Harris and Sans, 1967	Carrot
Aldrin	5.66	66.50	364.9	C1C2C=CC1C3C2C4(C(=C(C3(C4(Cl)Cl)Cl)Cl)Cl)Cl	0.24	1.35	-2.92	Harris and Sans, 1967	Carrot
Dieldrin	4.55	1.40	380.9	C1C2C3C(C1C4C2O4)C5(C(=C(C3(C5(Cl)Cl)Cl)Cl)Cl)Cl	0.24	1.23	-0.60	Harris and Sans, 1967	Carrot
Dieldrin	4.55	3.60	380.9	C1C2C3C(C1C4C2O4)C5(C(=C(C3(C5(Cl)Cl)Cl)Cl)Cl)Cl	0.24	1.25	-0.99	Harris and Sans, 1967	Carrot
Dieldrin	4.55	66.50	380.9	C1C2C3C(C1C4C2O4)C5(C(=C(C3(C5(Cl)Cl)Cl)Cl)Cl)Cl	0.24	1.22	-2.29	Harris and Sans, 1967	Carrot
Dieldrin	4.55	3.60	380.9	C1C2C3C(C1C4C2O4)C5(C(=C(C3(C5(Cl)Cl)Cl)Cl)Cl)Cl	0.10	0.91	-1.33	Harris and Sans, 1967	Radish
Dieldrin	4.55	66.50	380.9	C1C2C3C(C1C4C2O4)C5(C(=C(C3(C5(Cl)Cl)Cl)Cl)Cl)Cl	0.10	0.92	-2.59	Harris and Sans, 1967	Radish

Dieldrin	4.55	3.60	380.9	C1C2C3C(C1C4C2O4)C5(C(=C(C3(C5(Cl)Cl)Cl)Cl)Cl)Cl	0.10	0.69	-1.56	Harris and Sans, 1967	Turnips
m-DCB (1,3-DCB)	3.44	2.82	147	C1=CC(=CC(=C1)Cl)Cl	0.34	1.00	0.22	Zhang et al., 2005	Spinach
m-DCB (1,3-DCB)	3.44	0.78	147	C1=CC(=CC(=C1)Cl)Cl	0.34	0.83	0.61	Zhang et al., 2005	Spinach
m-DCB (1,3-DCB)	3.44	1.41	147	C1=CC(=CC(=C1)Cl)Cl	0.24	0.45	-0.03	Zhang et al., 2005	Carrot
m-DCB (1,3-DCB)	3.44	0.78	147	C1=CC(=CC(=C1)Cl)Cl	0.24	0.11	-0.12	Zhang et al., 2005	Carrot
m-DCB (1,3-DCB)	3.44	2.82	147	C1=CC(=CC(=C1)Cl)Cl	0.09	0.19	-0.59	Zhang et al., 2005	Radish
m-DCB (1,3-DCB)	3.44	0.78	147	C1=CC(=CC(=C1)Cl)Cl	0.09	0.07	-0.15	Zhang et al., 2005	Radish
p-DCB (1,4-DCB)	3.37	2.82	147	C1=CC(=CC=C1Cl)Cl	0.34	0.85	0.14	Zhang et al., 2005	Spinach
p-DCB (1,4-DCB)	3.37	1.41	147	C1=CC(=CC=C1Cl)Cl	0.34	0.29	-0.12	Zhang et al., 2005	Spinach
p-DCB (1,4-DCB)	3.37	1.41	147	C1=CC(=CC=C1Cl)Cl	0.09	0.04	-0.38	Zhang et al., 2005	Radish
o-DCB (1,2-DCB)	3.38	0.78	147	C1=CC=C(C(=C1)Cl)Cl	0.34	0.87	0.70	Zhang et al., 2005	Spinach
o-DCB (1,2-DCB)	3.38	0.78	147	C1=CC=C(C(=C1)Cl)Cl	0.24	0.17	0.00	Zhang et al., 2005	Carrot
o-DCB (1,2-DCB)	3.38	0.78	147	C1=CC=C(C(=C1)Cl)Cl	0.09	-0.01	-0.18	Zhang et al., 2005	Radish
1,2,4-TCB	4.02	2.82	181.4	C1=CC(=C(C=C1Cl)Cl)Cl	0.34	0.90	-0.41	Zhang et al., 2005	Spinach
1,2,4-TCB	4.02	1.41	181.4	C1=CC(=C(C=C1Cl)Cl)Cl	0.34	0.90	-0.10	Zhang et al., 2005	Spinach

1,2,4-TCB	4.02	2.82	181.4	C1=CC(=C(C=C1Cl)Cl)Cl	0.17	0.96	-0.35	Zhang et al., 2005	Celery
1,2,4-TCB	4.02	1.41	181.4	C1=CC(=C(C=C1Cl)Cl)Cl	0.17	0.81	-0.20	Zhang et al., 2005	Celery
1,2,4-TCB	4.02	0.78	181.4	C1=CC(=C(C=C1Cl)Cl)Cl	0.17	0.67	-0.08	Zhang et al., 2005	Celery
1,2,4-TCB	4.02	1.41	181.4	C1=CC(=C(C=C1Cl)Cl)Cl	0.24	0.59	-0.41	Zhang et al., 2005	Carrot
1,2,4-TCB	4.02	2.82	181.4	C1=CC(=C(C=C1Cl)Cl)Cl	0.09	0.36	-0.94	Zhang et al., 2005	Radish
1,2,4-TCB	4.02	1.41	181.4	C1=CC(=C(C=C1Cl)Cl)Cl	0.09	0.24	-0.76	Zhang et al., 2005	Radish
Fluorene	4.18	12.72	166.22	C1C2=CC=CC=C2C3=CC=CC=C31	0.10	0.92	-1.59	Cai et al., 2008	Radish
Phenanthrene	4.46	12.72	178.23	C1=CC=C2C(=C1)C=CC3=CC=CC=C32	0.10	1.34	-1.45	Cai et al., 2008	Radish
Phenanthrene	4.46	4.84	178.23	C1=CC=C2C(=C1)C=CC3=CC=CC=C32	0.10	1.32	-1.05	Cai et al., 2008	Radish
Anthracene	4.54	3.78	178.23	C1=CC=C2C=C3C=CC=CC3=CC2=C1	0.10	0.71	-1.63	Cai et al., 2008	Radish
Anthracene	4.54	12.72	178.23	C1=CC=C2C=C3C=CC=CC3=CC2=C1	0.10	0.71	-2.15	Cai et al., 2008	Radish
Fluoranthene	5.16	0.79	202.25	C1=CC=C2C(=C1)C3=CC=CC4=C3C2=CC=C4	0.10	1.56	-0.72	Cai et al., 2008	Radish
Benzo[a]pyrene	6.34	3.78	252.3	C1=CC=C2C3=C4C(=CC2=C1)C=CC5=C4C(=CC=C5)C=C3	0.10	1.62	-2.52	Cai et al., 2008	Radish
Di(2-ethylhexyl) phthalate	7.60	6.76	390.6	CCCCC(CC)COC(=O)C1=CC=CC=C1C(=O)OCC(CC)CCCC	0.10	2.80	-1.94	Cai et al., 2008	Radish
Di(2-ethylhexyl) phthalate	7.60	12.72	390.6	CCCCC(CC)COC(=O)C1=CC=CC=C1C(=O)OCC(CC)CCCC	0.10	2.98	-2.40	Cai et al., 2008	Radish
Phenanthrene	4.46	1.45	178.23	C1=CC=C2C(=C1)C=CC3=CC=CC=C32	0.32	0.57	-1.27	Gao et al., 2005	Ryegrass

Phenanthrene	4.46	1.45	178.23	C1=CC=C2C(=C1)C=CC3=CC=CC=C32	0.68	0.96	-0.88	Gao et al., 2005	Chinese cabbage
Phenanthrene	4.46	1.45	178.23	C1=CC=C2C(=C1)C=CC3=CC=CC=C32	0.32	0.70	-1.15	Gao et al., 2005	Amaranth
Pyrene	5.18	1.45	202.25	C1=CC2=C3C(=C1)C=CC4=CC=CC(=C43)C=C2	0.32	1.51	-1.05	Gao et al., 2005	Ryegrass
Pyrene	5.18	1.45	202.25	C1=CC2=C3C(=C1)C=CC4=CC=CC(=C43)C=C2	0.68	2.31	-0.26	Gao et al., 2005	Chinese cabbage
alpha-HCH	3.81	6.36	290.83	C1(C(C(C(C(C1Cl)Cl)Cl)Cl)Cl)Cl	0.10	-0.74	-2.20	Mikes et al., 2009	Radish
HCB	5.50	6.36	284.8	C1(=C(C(=C(C(=C1Cl)Cl)Cl)Cl)Cl)Cl	0.10	0.95	-2.11	Mikes et al., 2009	Radish
o,p'-DDE	5.76	6.36	318	C1=CC=C(C(=C1)C(=C(Cl)Cl)C2=CC=C(C=C2)Cl)Cl	0.10	1.74	-1.49	Mikes et al., 2009	Radish
p,p'-DDE	5.91	6.36	318	C1=CC(=CC=C1C(=C(Cl)Cl)C2=CC=C(C=C2)Cl)Cl	0.10	2.03	-1.24	Mikes et al., 2009	Radish
o,p'-DDD	5.82	6.36	320	C1=CC=C(C(=C1)C(C2=CC=C(C=C2)Cl)C(Cl)Cl)Cl	0.10	2.03	-1.25	Mikes et al., 2009	Radish
p,p'-DDD	5.69	6.36	320	C1=CC(=CC=C1C(C2=CC=C(C=C2)Cl)C(Cl)Cl)Cl	0.10	2.12	-1.05	Mikes et al., 2009	Radish
o,p'-DDT	6.19	6.36	354.5	C1=CC=C(C(=C1)C(C2=CC=C(C=C2)Cl)C(Cl)(Cl)Cl)Cl	0.10	2.32	-1.30	Mikes et al., 2009	Radish
p,p'-DDT	5.98	6.36	354.5	C1=CC(=CC=C1C(C2=CC=C(C=C2)Cl)C(Cl)(Cl)Cl)Cl	0.10	2.40	-1.74	Mikes et al., 2009	Radish
PCB 101	6.50	6.36	326.4	C1=CC(=C(C=C1Cl)C2=CC(=C(C=C2Cl)Cl)Cl)Cl	0.10	2.32	-1.72	Mikes et al., 2009	Radish
PCB 153	6.90	6.36	360.9	C1=C(C(=CC(=C1Cl)Cl)Cl)C2=CC(=C(C=C2Cl)Cl)Cl	0.10	2.48	-2.03	Mikes et al., 2009	Radish
PCB 138	6.69	6.36	360.9	C1=CC(=C(C(=C1C2=CC(=C(C=C2Cl)Cl)Cl)Cl)Cl)Cl	0.10	2.26	-2.09	Mikes et al., 2009	Radish

PCB 180	7.20	6.36	395.3	C1=C(C(=CC(=C1Cl)Cl)Cl)C2=CC(=C(C(=C2Cl)Cl)Cl)Cl	0.10	2.40	-2.07	Mikes et al., 2009	Radish
BDE-100	7.24	3.19	564.7	C1=CC(=C(C=C1Br)Br)OC2=C(C=C(C=C2Br)Br)Br	0.53	2.61	-1.66	Huang et al., 2011	Maize
BDE-100	7.24	3.19	564.7	C1=CC(=C(C=C1Br)Br)OC2=C(C=C(C=C2Br)Br)Br	0.56	2.76	-1.51	Huang et al., 2011	Ryegrass
BDE-100	7.24	1.90	564.7	C1=CC(=C(C=C1Br)Br)OC2=C(C=C(C=C2Br)Br)Br	0.70	2.88	-1.17	Huang et al., 2011	Pumpkin
BDE-100	7.24	1.90	564.7	C1=CC(=C(C=C1Br)Br)OC2=C(C=C(C=C2Br)Br)Br	0.53	2.84	-1.21	Huang et al., 2011	Maize
BDE-100	7.24	1.90	564.7	C1=CC(=C(C=C1Br)Br)OC2=C(C=C(C=C2Br)Br)Br	0.56	2.67	-1.37	Huang et al., 2011	Ryegrass
BDE-100	7.24	0.98	564.7	C1=CC(=C(C=C1Br)Br)OC2=C(C=C(C=C2Br)Br)Br	0.70	2.69	-1.07	Huang et al., 2011	Pumpkin
BDE-100	7.24	0.98	564.7	C1=CC(=C(C=C1Br)Br)OC2=C(C=C(C=C2Br)Br)Br	0.53	2.70	-1.05	Huang et al., 2011	Maize
BDE-100	7.24	0.98	564.7	C1=CC(=C(C=C1Br)Br)OC2=C(C=C(C=C2Br)Br)Br	0.56	2.84	-0.92	Huang et al., 2011	Ryegrass
BDE-153	7.90	3.19	643.6	C1=C(C(=CC(=C1Br)Br)Br)OC2=CC(=C(C=C2Br)Br)Br	0.70	2.95	-1.92	Huang et al., 2011	Pumpkin
BDE-153	7.90	3.19	643.6	C1=C(C(=CC(=C1Br)Br)Br)OC2=CC(=C(C=C2Br)Br)Br	0.56	3.64	-1.23	Huang et al., 2011	Ryegrass
BDE-153	7.90	1.90	643.6	C1=C(C(=CC(=C1Br)Br)Br)OC2=CC(=C(C=C2Br)Br)Br	0.70	3.19	-1.45	Huang et al., 2011	Pumpkin
BDE-153	7.90	1.90	643.6	C1=C(C(=CC(=C1Br)Br)Br)OC2=CC(=C(C=C2Br)Br)Br	0.53	3.39	-1.25	Huang et al., 2011	Maize
BDE-153	7.90	1.90	643.6	C1=C(C(=CC(=C1Br)Br)Br)OC2=CC(=C(C=C2Br)Br)Br	0.56	3.37	-1.27	Huang et al., 2011	Ryegrass

BDE-153	7.90	0.98	643.6	C1=C(C(=CC(=C1Br)Br)Br)OC2=CC(=C(C=C2Br)Br)Br	0.70	3.30	-1.05	Huang et al., 2011	Pumpkin
BDE-153	7.90	0.98	643.6	C1=C(C(=CC(=C1Br)Br)Br)OC2=CC(=C(C=C2Br)Br)Br	0.53	3.34	-1.01	Huang et al., 2011	Maize
BDE-153	7.90	0.98	643.6	C1=C(C(=CC(=C1Br)Br)Br)OC2=CC(=C(C=C2Br)Br)Br	0.56	3.14	-1.21	Huang et al., 2011	Ryegrass
BDE-154	7.82	3.19	643.6	C1=C(C=C(C(=C1Br)OC2=CC(=C(C=C2Br)Br)Br)Br)Br	0.70	3.52	-1.27	Huang et al., 2011	Pumpkin
BDE-154	7.82	3.19	643.6	C1=C(C=C(C(=C1Br)OC2=CC(=C(C=C2Br)Br)Br)Br)Br	0.53	3.59	-1.20	Huang et al., 2011	Maize
BDE-154	7.82	1.90	643.6	C1=C(C=C(C(=C1Br)OC2=CC(=C(C=C2Br)Br)Br)Br)Br	0.70	3.34	-1.23	Huang et al., 2011	Pumpkin
BDE-154	7.82	1.90	643.6	C1=C(C=C(C(=C1Br)OC2=CC(=C(C=C2Br)Br)Br)Br)Br	0.53	3.24	-1.33	Huang et al., 2011	Maize
BDE-154	7.82	1.90	643.6	C1=C(C=C(C(=C1Br)OC2=CC(=C(C=C2Br)Br)Br)Br)Br	0.56	3.16	-1.41	Huang et al., 2011	Ryegrass
BDE-154	7.82	0.98	643.6	C1=C(C=C(C(=C1Br)OC2=CC(=C(C=C2Br)Br)Br)Br)Br	0.70	3.14	-1.15	Huang et al., 2011	Pumpkin
BDE-154	7.82	0.98	643.6	C1=C(C=C(C(=C1Br)OC2=CC(=C(C=C2Br)Br)Br)Br)Br	0.53	3.22	-1.06	Huang et al., 2011	Maize
BDE-154	7.82	0.98	643.6	C1=C(C=C(C(=C1Br)OC2=CC(=C(C=C2Br)Br)Br)Br)Br	0.56	3.14	-1.14	Huang et al., 2011	Ryegrass
BDE-17	5.74	3.19	406.89	C1=CC=C(C(=C1)OC2=C(C=C(C=C2)Br)Br)Br	0.70	1.82	-1.09	Huang et al., 2011	Pumpkin
BDE-17	5.74	3.19	406.89	C1=CC=C(C(=C1)OC2=C(C=C(C=C2)Br)Br)Br	0.53	1.84	-1.08	Huang et al., 2011	Maize
BDE-17	5.74	3.19	406.89	C1=CC=C(C(=C1)OC2=C(C=C(C=C2)Br)Br)Br	0.56	1.68	-1.24	Huang et al., 2011	Ryegrass

BDE-17	5.74	1.90	406.89	C1=CC=C(C(=C1)OC2=C(C=C(C=C2)Br)Br)Br	0.70	1.59	-1.10	Huang et al., 2011	Pumpkin
BDE-17	5.74	1.90	406.89	C1=CC=C(C(=C1)OC2=C(C=C(C=C2)Br)Br)Br	0.53	1.66	-1.03	Huang et al., 2011	Maize
BDE-17	5.74	1.90	406.89	C1=CC=C(C(=C1)OC2=C(C=C(C=C2)Br)Br)Br	0.56	1.60	-1.09	Huang et al., 2011	Ryegrass
BDE-17	5.74	0.98	406.89	C1=CC=C(C(=C1)OC2=C(C=C(C=C2)Br)Br)Br	0.70	1.60	-0.80	Huang et al., 2011	Pumpkin
BDE-183	8.27	3.19	722.5	C1=C(C(=CC(=C1Br)Br)Br)OC2=C(C(=C(C=C2Br)Br)Br)Br	0.70	3.65	-1.55	Huang et al., 2011	Pumpkin
BDE-183	8.27	3.19	722.5	C1=C(C(=CC(=C1Br)Br)Br)OC2=C(C(=C(C=C2Br)Br)Br)Br	0.53	3.62	-1.59	Huang et al., 2011	Maize
BDE-183	8.27	3.19	722.5	C1=C(C(=CC(=C1Br)Br)Br)OC2=C(C(=C(C=C2Br)Br)Br)Br	0.56	3.83	-1.37	Huang et al., 2011	Ryegrass
BDE-183	8.27	1.90	722.5	C1=C(C(=CC(=C1Br)Br)Br)OC2=C(C(=C(C=C2Br)Br)Br)Br	0.70	3.81	-1.17	Huang et al., 2011	Pumpkin
BDE-183	8.27	1.90	722.5	C1=C(C(=CC(=C1Br)Br)Br)OC2=C(C(=C(C=C2Br)Br)Br)Br	0.53	4.02	-0.96	Huang et al., 2011	Maize
BDE-183	8.27	1.90	722.5	C1=C(C(=CC(=C1Br)Br)Br)OC2=C(C(=C(C=C2Br)Br)Br)Br	0.56	3.95	-1.02	Huang et al., 2011	Ryegrass
BDE-183	8.27	0.98	722.5	C1=C(C(=CC(=C1Br)Br)Br)OC2=C(C(=C(C=C2Br)Br)Br)Br	0.70	2.99	-1.70	Huang et al., 2011	Pumpkin
BDE-183	8.27	0.98	722.5	C1=C(C(=CC(=C1Br)Br)Br)OC2=C(C(=C(C=C2Br)Br)Br)Br	0.53	3.17	-1.52	Huang et al., 2011	Maize
BDE-183	8.27	0.98	722.5	C1=C(C(=CC(=C1Br)Br)Br)OC2=C(C(=C(C=C2Br)Br)Br)Br	0.56	3.19	-1.50	Huang et al., 2011	Ryegrass
BDE-206	8.47	3.19	880.3	C1=C(C(=C(C(=C1Br)Br)Br)Br)OC2=C(C(=C(C(=C2Br)Br)Br)Br)Br	0.70	4.26	-1.12	Huang et al., 2011	Pumpkin

BDE-206	8.47	3.19	880.3	C1=C(C(=C(C(=C1Br)Br)Br)OC2=C(C(=C(C(=C2Br)Br)Br)Br)Br	0.53	4.43	-0.95	Huang et al., 2011	Maize
BDE-206	8.47	3.19	880.3	C1=C(C(=C(C(=C1Br)Br)Br)OC2=C(C(=C(C(=C2Br)Br)Br)Br)Br	0.56	3.78	-1.60	Huang et al., 2011	Ryegrass
BDE-206	8.47	1.90	880.3	C1=C(C(=C(C(=C1Br)Br)Br)OC2=C(C(=C(C(=C2Br)Br)Br)Br)Br	0.70	3.13	-1.74	Huang et al., 2011	Pumpkin
BDE-206	8.47	1.90	880.3	C1=C(C(=C(C(=C1Br)Br)Br)OC2=C(C(=C(C(=C2Br)Br)Br)Br)Br	0.53	3.37	-1.50	Huang et al., 2011	Maize
BDE-206	8.47	1.90	880.3	C1=C(C(=C(C(=C1Br)Br)Br)OC2=C(C(=C(C(=C2Br)Br)Br)Br)Br	0.56	3.18	-1.69	Huang et al., 2011	Ryegrass
BDE-209	8.70	0.98	959.2	C1(=C(C(=C(C(=C1Br)Br)Br)Br)OC2=C(C(=C(C(=C2Br)Br)Br)Br)Br	0.70	4.31	-1.28	Huang et al., 2011	Pumpkin
BDE-209	8.70	3.19	959.2	C1(=C(C(=C(C(=C1Br)Br)Br)Br)OC2=C(C(=C(C(=C2Br)Br)Br)Br)Br	0.53	4.11	-1.48	Huang et al., 2011	Maize
BDE-209	8.70	3.19	959.2	C1(=C(C(=C(C(=C1Br)Br)Br)Br)OC2=C(C(=C(C(=C2Br)Br)Br)Br)Br	0.56	4.21	-1.38	Huang et al., 2011	Ryegrass
BDE-209	8.70	1.90	959.2	C1(=C(C(=C(C(=C1Br)Br)Br)Br)OC2=C(C(=C(C(=C2Br)Br)Br)Br)Br	0.70	3.86	-1.50	Huang et al., 2011	Pumpkin
BDE-209	8.70	1.90	959.2	C1(=C(C(=C(C(=C1Br)Br)Br)Br)OC2=C(C(=C(C(=C2Br)Br)Br)Br)Br	0.53	3.82	-1.54	Huang et al., 2011	Maize
BDE-209	8.70	1.90	959.2	C1(=C(C(=C(C(=C1Br)Br)Br)Br)OC2=C(C(=C(C(=C2Br)Br)Br)Br)Br	0.56	3.72	-1.64	Huang et al., 2011	Ryegrass
BDE-28	5.94	3.19	406.89	C1=CC(=CC=C1OC2=C(C=C(C=C2)Br)Br)Br	0.53	1.96	-1.13	Huang et al., 2011	Maize
BDE-28	5.94	1.90	406.89	C1=CC(=CC=C1OC2=C(C=C(C=C2)Br)Br)Br	0.53	1.95	-0.92	Huang et al., 2011	Maize
BDE-28	5.94	1.90	406.89	C1=CC(=CC=C1OC2=C(C=C(C=C2)Br)Br)Br	0.56	2.07	-0.80	Huang et al., 2011	Ryegrass

BDE-47	6.81	3.19	485.79	C1=CC(=C(C=C1Br)Br)OC2=C(C=C(C=C2)Br)Br	0.70	3.09	-0.80	Huang et al., 2011	Pumpkin
BDE-47	6.81	3.19	485.79	C1=CC(=C(C=C1Br)Br)OC2=C(C=C(C=C2)Br)Br	0.53	3.00	-0.88	Huang et al., 2011	Maize
BDE-47	6.81	3.19	485.79	C1=CC(=C(C=C1Br)Br)OC2=C(C=C(C=C2)Br)Br	0.56	2.99	-0.89	Huang et al., 2011	Ryegrass
BDE-47	6.81	1.90	485.79	C1=CC(=C(C=C1Br)Br)OC2=C(C=C(C=C2)Br)Br	0.70	3.02	-0.64	Huang et al., 2011	Pumpkin
BDE-47	6.81	1.90	485.79	C1=CC(=C(C=C1Br)Br)OC2=C(C=C(C=C2)Br)Br	0.53	2.90	-0.75	Huang et al., 2011	Maize
BDE-47	6.81	1.90	485.79	C1=CC(=C(C=C1Br)Br)OC2=C(C=C(C=C2)Br)Br	0.56	2.92	-0.73	Huang et al., 2011	Ryegrass
BDE-47	6.81	0.98	485.79	C1=CC(=C(C=C1Br)Br)OC2=C(C=C(C=C2)Br)Br	0.70	2.45	-0.92	Huang et al., 2011	Pumpkin
BDE-47	6.81	0.98	485.79	C1=CC(=C(C=C1Br)Br)OC2=C(C=C(C=C2)Br)Br	0.53	2.32	-1.05	Huang et al., 2011	Maize
BDE-99	7.32	3.19	564.7	C1=CC(=C(C=C1Br)Br)OC2=CC(=C(C=C2Br)Br)Br	0.70	3.27	-1.07	Huang et al., 2011	Pumpkin
BDE-99	7.32	3.19	564.7	C1=CC(=C(C=C1Br)Br)OC2=CC(=C(C=C2Br)Br)Br	0.53	3.26	-1.08	Huang et al., 2011	Maize
BDE-99	7.32	3.19	564.7	C1=CC(=C(C=C1Br)Br)OC2=CC(=C(C=C2Br)Br)Br	0.56	3.23	-1.11	Huang et al., 2011	Ryegrass
BDE-99	7.32	1.90	564.7	C1=CC(=C(C=C1Br)Br)OC2=CC(=C(C=C2Br)Br)Br	0.70	3.21	-0.90	Huang et al., 2011	Pumpkin
BDE-99	7.32	1.90	564.7	C1=CC(=C(C=C1Br)Br)OC2=CC(=C(C=C2Br)Br)Br	0.53	3.06	-1.06	Huang et al., 2011	Maize
BDE-99	7.32	1.90	564.7	C1=CC(=C(C=C1Br)Br)OC2=CC(=C(C=C2Br)Br)Br	0.56	2.85	-1.27	Huang et al., 2011	Ryegrass

BDE-99	7.32	0.98	564.7	C1=CC(=C(C=C1Br)Br)OC2=CC(=C(C=C2Br)Br)Br	0.70	2.85	-0.98	Huang et al., 2011	Pumpkin
BDE-99	7.32	0.98	564.7	C1=CC(=C(C=C1Br)Br)OC2=CC(=C(C=C2Br)Br)Br	0.53	2.78	-1.05	Huang et al., 2011	Maize
BDE-99	7.32	0.98	564.7	C1=CC(=C(C=C1Br)Br)OC2=CC(=C(C=C2Br)Br)Br	0.56	2.94	-0.88	Huang et al., 2011	Ryegrass
alpha-HBCD	5.38	1.85	641.7	C1C[C@H]([C@H](CC[C@H]([C@@H](CC[C@@H]([C@@H]1Br)Br)Br)Br)Br)Br	1.10	1.74	-0.61	Zhu et al., 2016	Wheat
Dieldrin	4.55	13.28	380.9	C1C2C3C(C1C4C2O4)C5(C(=C(C3(C5(Cl)Cl)Cl)Cl)Cl)Cl	0.53	1.99	-0.82	Beestman et al., 1969	Maize
Dieldrin	4.55	0.69	380.9	C1C2C3C(C1C4C2O4)C5(C(=C(C3(C5(Cl)Cl)Cl)Cl)Cl)Cl	0.53	2.03	0.52	Beestman et al., 1969	Maize
Dieldrin	4.55	0.86	380.9	C1C2C3C(C1C4C2O4)C5(C(=C(C3(C5(Cl)Cl)Cl)Cl)Cl)Cl	0.53	2.01	0.38	Beestman et al., 1969	Maize
Dieldrin	4.55	6.55	380.9	C1C2C3C(C1C4C2O4)C5(C(=C(C3(C5(Cl)Cl)Cl)Cl)Cl)Cl	0.53	1.96	-0.54	Beestman et al., 1969	Maize
Dieldrin	4.55	1.21	380.9	C1C2C3C(C1C4C2O4)C5(C(=C(C3(C5(Cl)Cl)Cl)Cl)Cl)Cl	0.53	2.00	0.22	Beestman et al., 1969	Maize
Dieldrin	4.55	8.97	380.9	C1C2C3C(C1C4C2O4)C5(C(=C(C3(C5(Cl)Cl)Cl)Cl)Cl)Cl	0.53	2.01	-0.64	Beestman et al., 1969	Maize
1,4-DCB	3.37	3.55	147	C1=CC(=CC=C1Cl)Cl	1.00	1.72	1.03	Scheunert et al., 1994	Barely
1,2,4-TCB	4.02	3.55	181.4	C1=CC(=C(C=C1Cl)Cl)Cl	1.00	1.98	0.65	Scheunert et al., 1994	Barely
1,2,3,5-TeCB	4.59	3.55	215.9	C1=C(C=C(C(=C1Cl)Cl)Cl)Cl	1.00	2.39	0.75	Scheunert et al., 1994	Barely

Pentachlorobeneze	5.03	3.55	250.3	C1=C(C(=C(C(=C1Cl)Cl)Cl)Cl)Cl	1.00	2.07	0.03	Scheunert et al., 1994	Barely
Hexachlorobenze	5.50	3.55	284.8	C1(=C(C(=C(C(=C1Cl)Cl)Cl)Cl)Cl)Cl	1.00	2.27	-0.09	Scheunert et al., 1994	Barely
Naphthalene	3.36	5.31	128.17	C1=CC=C2C=CC=CC2=C1	1.14	0.88	-0.42	Tao et al., 2009	Wheat
Naphthalene	3.36	1.41	128.17	C1=CC=C2C=CC=CC2=C1	1.14	0.72	-0.01	Tao et al., 2009	Wheat
Naphthalene	3.36	4.33	128.17	C1=CC=C2C=CC=CC2=C1	1.14	1.06	-0.16	Tao et al., 2009	Wheat
Naphthalene	3.36	2.71	128.17	C1=CC=C2C=CC=CC2=C1	1.14	1.18	0.17	Tao et al., 2009	Wheat
Naphthalene	3.36	5.71	128.17	C1=CC=C2C=CC=CC2=C1	1.14	0.73	-0.61	Tao et al., 2009	Wheat
Naphthalene	3.36	2.60	128.17	C1=CC=C2C=CC=CC2=C1	1.14	0.98	-0.02	Tao et al., 2009	Wheat
Naphthalene	3.36	4.81	128.17	C1=CC=C2C=CC=CC2=C1	1.14	0.82	-0.44	Tao et al., 2009	Wheat
Naphthalene	3.36	2.67	128.17	C1=CC=C2C=CC=CC2=C1	1.14	0.84	-0.17	Tao et al., 2009	Wheat
Naphthalene	3.36	4.74	128.17	C1=CC=C2C=CC=CC2=C1	1.14	1.08	-0.18	Tao et al., 2009	Wheat
Naphthalene	3.36	4.16	128.17	C1=CC=C2C=CC=CC2=C1	1.14	1.10	-0.10	Tao et al., 2009	Wheat
Acenaphthene	3.92	4.33	154.21	C1CC2=CC=CC3=C2C1=CC=C3	1.14	1.67	-0.11	Tao et al., 2009	Wheat
Acenaphthene	3.92	2.71	154.21	C1CC2=CC=CC3=C2C1=CC=C3	1.14	1.56	-0.02	Tao et al., 2009	Wheat
Acenaphthene	3.92	5.71	154.21	C1CC2=CC=CC3=C2C1=CC=C3	1.14	1.21	-0.68	Tao et al., 2009	Wheat
Acenaphthene	3.92	2.60	154.21	C1CC2=CC=CC3=C2C1=CC=C3	1.14	1.47	-0.09	Tao et al., 2009	Wheat
Acenaphthene	3.92	3.47	154.21	C1CC2=CC=CC3=C2C1=CC=C3	1.14	1.16	-0.53	Tao et al., 2009	Wheat
Acenaphthene	3.92	5.31	154.21	C1CC2=CC=CC3=C2C1=CC=C3	1.14	1.49	-0.38	Tao et al., 2009	Wheat
Acenaphthene	3.92	3.47	154.21	C1CC2=CC=CC3=C2C1=CC=C3	1.14	1.23	-0.46	Tao et al., 2009	Wheat
Acenaphthene	3.92	6.22	154.21	C1CC2=CC=CC3=C2C1=CC=C3	1.14	1.26	-0.68	Tao et al., 2009	Wheat
Acenaphthene	3.92	4.81	154.21	C1CC2=CC=CC3=C2C1=CC=C3	1.14	1.51	-0.31	Tao et al., 2009	Wheat

Acenaphthene	3.92	2.67	154.21	C1CC2=CC=CC3=C2C1=CC=C3	1.14	1.39	-0.18	Tao et al., 2009	Wheat
Acenaphthene	3.92	4.74	154.21	C1CC2=CC=CC3=C2C1=CC=C3	1.14	1.57	-0.25	Tao et al., 2009	Wheat
Acenaphthene	3.92	4.16	154.21	C1CC2=CC=CC3=C2C1=CC=C3	1.14	1.37	-0.39	Tao et al., 2009	Wheat
Fluorene	4.18	1.41	166.22	C1C2=CC=CC=C2C3=CC=CC=C31	1.14	1.51	-0.04	Tao et al., 2009	Wheat
Fluorene	4.18	4.33	166.22	C1C2=CC=CC=C2C3=CC=CC=C31	1.14	1.76	-0.28	Tao et al., 2009	Wheat
Fluorene	4.18	5.71	166.22	C1C2=CC=CC=C2C3=CC=CC=C31	1.14	1.61	-0.55	Tao et al., 2009	Wheat
Fluorene	4.18	3.47	166.22	C1C2=CC=CC=C2C3=CC=CC=C31	1.14	1.59	-0.35	Tao et al., 2009	Wheat
Fluorene	4.18	5.31	166.22	C1C2=CC=CC=C2C3=CC=CC=C31	1.14	1.73	-0.40	Tao et al., 2009	Wheat
Fluorene	4.18	3.47	166.22	C1C2=CC=CC=C2C3=CC=CC=C31	1.14	1.46	-0.48	Tao et al., 2009	Wheat
Fluorene	4.18	6.22	166.22	C1C2=CC=CC=C2C3=CC=CC=C31	1.14	1.53	-0.66	Tao et al., 2009	Wheat
Fluorene	4.18	4.81	166.22	C1C2=CC=CC=C2C3=CC=CC=C31	1.14	1.88	-0.20	Tao et al., 2009	Wheat
Fluorene	4.18	2.67	166.22	C1C2=CC=CC=C2C3=CC=CC=C31	1.14	1.71	-0.12	Tao et al., 2009	Wheat
Fluorene	4.18	4.16	166.22	C1C2=CC=CC=C2C3=CC=CC=C31	1.14	1.72	-0.30	Tao et al., 2009	Wheat
Phenanthrene	4.46	5.31	178.23	C1=CC=C2C(=C1)C=CC3=CC=CC=C32	1.14	1.67	-0.74	Tao et al., 2009	Wheat
Phenanthrene	4.46	1.41	178.23	C1=CC=C2C(=C1)C=CC3=CC=CC=C32	1.14	1.67	-0.16	Tao et al., 2009	Wheat
Phenanthrene	4.46	4.33	178.23	C1=CC=C2C(=C1)C=CC3=CC=CC=C32	1.14	2.05	-0.27	Tao et al., 2009	Wheat
Phenanthrene	4.46	2.71	178.23	C1=CC=C2C(=C1)C=CC3=CC=CC=C32	1.14	1.98	-0.14	Tao et al., 2009	Wheat
Phenanthrene	4.46	5.71	178.23	C1=CC=C2C(=C1)C=CC3=CC=CC=C32	1.14	1.64	-0.80	Tao et al., 2009	Wheat
Phenanthrene	4.46	2.60	178.23	C1=CC=C2C(=C1)C=CC3=CC=CC=C32	1.14	1.96	-0.14	Tao et al., 2009	Wheat

Phenanthrene	4.46	3.47	178.23	C1=CC=C2C(=C1)C=CC3=CC=CC=C32	1.14	1.68	-0.54	Tao et al., 2009	Wheat
Phenanthrene	4.46	5.31	178.23	C1=CC=C2C(=C1)C=CC3=CC=CC=C32	1.14	1.85	-0.56	Tao et al., 2009	Wheat
Phenanthrene	4.46	6.22	178.23	C1=CC=C2C(=C1)C=CC3=CC=CC=C32	1.14	1.75	-0.72	Tao et al., 2009	Wheat
Phenanthrene	4.46	4.81	178.23	C1=CC=C2C(=C1)C=CC3=CC=CC=C32	1.14	2.01	-0.36	Tao et al., 2009	Wheat
Phenanthrene	4.46	2.67	178.23	C1=CC=C2C(=C1)C=CC3=CC=CC=C32	1.14	1.89	-0.22	Tao et al., 2009	Wheat
Phenanthrene	4.46	4.74	178.23	C1=CC=C2C(=C1)C=CC3=CC=CC=C32	1.14	1.89	-0.47	Tao et al., 2009	Wheat
Phenanthrene	4.46	4.16	178.23	C1=CC=C2C(=C1)C=CC3=CC=CC=C32	1.14	1.89	-0.41	Tao et al., 2009	Wheat
Anthracene	4.54	5.31	178.23	C1=CC=C2C=C3C=CC=CC3=CC2=C1	1.14	1.62	-0.87	Tao et al., 2009	Wheat
Anthracene	4.54	1.41	178.23	C1=CC=C2C=C3C=CC=CC3=CC2=C1	1.14	1.69	-0.22	Tao et al., 2009	Wheat
Anthracene	4.54	2.71	178.23	C1=CC=C2C=C3C=CC=CC3=CC2=C1	1.14	1.95	-0.24	Tao et al., 2009	Wheat
Anthracene	4.54	5.71	178.23	C1=CC=C2C=C3C=CC=CC3=CC2=C1	1.14	1.82	-0.70	Tao et al., 2009	Wheat
Anthracene	4.54	2.60	178.23	C1=CC=C2C=C3C=CC=CC3=CC2=C1	1.14	1.67	-0.51	Tao et al., 2009	Wheat
Anthracene	4.54	3.47	178.23	C1=CC=C2C=C3C=CC=CC3=CC2=C1	1.14	1.97	-0.34	Tao et al., 2009	Wheat
Anthracene	4.54	5.31	178.23	C1=CC=C2C=C3C=CC=CC3=CC2=C1	1.14	2.10	-0.39	Tao et al., 2009	Wheat
Anthracene	4.54	3.47	178.23	C1=CC=C2C=C3C=CC=CC3=CC2=C1	1.14	1.35	-0.95	Tao et al., 2009	Wheat
Anthracene	4.54	6.22	178.23	C1=CC=C2C=C3C=CC=CC3=CC2=C1	1.14	1.89	-0.66	Tao et al., 2009	Wheat
Anthracene	4.54	4.81	178.23	C1=CC=C2C=C3C=CC=CC3=CC2=C1	1.14	2.15	-0.29	Tao et al., 2009	Wheat
Anthracene	4.54	4.74	178.23	C1=CC=C2C=C3C=CC=CC3=CC2=C1	1.14	2.09	-0.35	Tao et al., 2009	Wheat

Anthracene	4.54	4.16	178.23	C1=CC=C2C=C3C=CC=CC3=CC2=C1	1.14	2.09	-0.29	Tao et al., 2009	Wheat
Fluoranthene	5.16	1.41	202.25	C1=CC=C2C(=C1)C3=CC=CC4=C3C2=CC=C4	1.14	2.54	0.01	Tao et al., 2009	Wheat
Fluoranthene	5.16	4.33	202.25	C1=CC=C2C(=C1)C3=CC=CC4=C3C2=CC=C4	1.14	2.59	-0.43	Tao et al., 2009	Wheat
Fluoranthene	5.16	5.71	202.25	C1=CC=C2C(=C1)C3=CC=CC4=C3C2=CC=C4	1.14	2.69	-0.45	Tao et al., 2009	Wheat
Fluoranthene	5.16	3.47	202.25	C1=CC=C2C(=C1)C3=CC=CC4=C3C2=CC=C4	1.14	2.66	-0.26	Tao et al., 2009	Wheat
Fluoranthene	5.16	5.31	202.25	C1=CC=C2C(=C1)C3=CC=CC4=C3C2=CC=C4	1.14	2.66	-0.45	Tao et al., 2009	Wheat
Pyrene	5.18	1.41	202.25	C1=CC2=C3C(=C1)C=CC4=CC=CC(=C43)C=C2	1.14	2.42	-0.13	Tao et al., 2009	Wheat
Pyrene	5.18	4.33	202.25	C1=CC2=C3C(=C1)C=CC4=CC=CC(=C43)C=C2	1.14	2.54	-0.50	Tao et al., 2009	Wheat
Pyrene	5.18	5.71	202.25	C1=CC2=C3C(=C1)C=CC4=CC=CC(=C43)C=C2	1.14	2.63	-0.53	Tao et al., 2009	Wheat
Pyrene	5.18	3.47	202.25	C1=CC2=C3C(=C1)C=CC4=CC=CC(=C43)C=C2	1.14	2.66	-0.28	Tao et al., 2009	Wheat
Pyrene	5.18	5.31	202.25	C1=CC2=C3C(=C1)C=CC4=CC=CC(=C43)C=C2	1.14	2.53	-0.60	Tao et al., 2009	Wheat
Pyrene	5.18	6.22	202.25	C1=CC2=C3C(=C1)C=CC4=CC=CC(=C43)C=C2	1.14	2.66	-0.53	Tao et al., 2009	Wheat
Benzo[a]anthracene	5.61	1.41	228.3	C1=CC=C2C(=C1)C=CC3=CC4=CC=CC=C4C=C32	1.14	3.09	0.11	Tao et al., 2009	Wheat
Benzo[a]anthracene	5.61	4.33	228.3	C1=CC=C2C(=C1)C=CC3=CC4=CC=CC=C4C=C32	1.14	3.03	-0.44	Tao et al., 2009	Wheat

Benzo[a]anthracene	5.61	5.31	228.3	C1=CC=C2C(=C1)C=CC3=CC4=CC=CC=C4C=C32	1.14	2.84	-0.72	Tao et al., 2009	Wheat
Benzo[a]anthracene	5.61	3.47	228.3	C1=CC=C2C(=C1)C=CC3=CC4=CC=CC=C4C=C32	1.14	3.03	-0.35	Tao et al., 2009	Wheat
Chrysene	5.73	5.31	228.3	C1=CC=C2C(=C1)C=CC3=C2C=CC4=CC=CC=C43	1.14	2.44	-1.23	Tao et al., 2009	Wheat
Chrysene	5.73	1.41	228.3	C1=CC=C2C(=C1)C=CC3=C2C=CC4=CC=CC=C43	1.14	3.18	0.08	Tao et al., 2009	Wheat
Chrysene	5.73	5.71	228.3	C1=CC=C2C(=C1)C=CC3=C2C=CC4=CC=CC=C43	1.14	3.19	-0.52	Tao et al., 2009	Wheat
Chrysene	5.73	3.47	228.3	C1=CC=C2C(=C1)C=CC3=C2C=CC4=CC=CC=C43	1.14	3.16	-0.33	Tao et al., 2009	Wheat
benzo[b]fluoranthene	5.78	3.47	252.3	C1=CC=C2C3=C4C(=CC=C3)C5=CC=CC=C5C4=CC2=C1	1.14	2.73	-0.81	Tao et al., 2009	Wheat
benzo[b]fluoranthene	5.78	6.22	252.3	C1=CC=C2C3=C4C(=CC=C3)C5=CC=CC=C5C4=CC2=C1	1.14	2.82	-0.98	Tao et al., 2009	Wheat
benzo[b]fluoranthene	5.78	4.81	252.3	C1=CC=C2C3=C4C(=CC=C3)C5=CC=CC=C5C4=CC2=C1	1.14	2.93	-0.76	Tao et al., 2009	Wheat
benzo[b]fluoranthene	5.78	2.67	252.3	C1=CC=C2C3=C4C(=CC=C3)C5=CC=CC=C5C4=CC2=C1	1.14	3.23	-0.20	Tao et al., 2009	Wheat
benzo[b]fluoranthene	5.78	4.16	252.3	C1=CC=C2C3=C4C(=CC=C3)C5=CC=CC=C5C4=CC2=C1	1.14	2.96	-0.66	Tao et al., 2009	Wheat
benzo[k]fluoranthene	6.20	4.33	252.3	C1=CC=C2C=C3C4=CC=CC5=C4C(=CC=C5)C3=CC2=C1	1.14	2.67	-1.39	Tao et al., 2009	Wheat
benzo[k]fluoranthene	6.20	2.71	252.3	C1=CC=C2C=C3C4=CC=CC5=C4C(=CC=C5)C3=CC2=C1	1.14	3.14	-0.71	Tao et al., 2009	Wheat
benzo[k]fluoranthene	6.20	5.71	252.3	C1=CC=C2C=C3C4=CC=CC5=C4C(=CC=C5)C3=CC2=C1	1.14	3.14	-1.04	Tao et al., 2009	Wheat

benzo[k]fluoranthene	6.20	3.47	252.3	C1=CC=C2C=C3C4=CC=CC5=C4C(=CC=C5)C3=CC2=C1	1.14	2.96	-1.00	Tao et al., 2009	Wheat
benzo[k]fluoranthene	6.20	5.31	252.3	C1=CC=C2C=C3C4=CC=CC5=C4C(=CC=C5)C3=CC2=C1	1.14	2.81	-1.33	Tao et al., 2009	Wheat
benzo[k]fluoranthene	6.20	3.47	252.3	C1=CC=C2C=C3C4=CC=CC5=C4C(=CC=C5)C3=CC2=C1	1.14	3.14	-0.82	Tao et al., 2009	Wheat
benzo[k]fluoranthene	6.20	6.22	252.3	C1=CC=C2C=C3C4=CC=CC5=C4C(=CC=C5)C3=CC2=C1	1.14	2.98	-1.23	Tao et al., 2009	Wheat
benzo[k]fluoranthene	6.20	4.74	252.3	C1=CC=C2C=C3C4=CC=CC5=C4C(=CC=C5)C3=CC2=C1	1.14	3.04	-1.05	Tao et al., 2009	Wheat
Benzo[a]pyrene	6.41	5.31	252.3	C1=CC=C2C3=C4C(=CC2=C1)C=CC5=C4C(=CC=C5)C=C3	1.14	2.71	-1.58	Tao et al., 2009	Wheat
Benzo[a]pyrene	6.41	4.33	252.3	C1=CC=C2C3=C4C(=CC2=C1)C=CC5=C4C(=CC=C5)C=C3	1.14	2.69	-1.51	Tao et al., 2009	Wheat
Benzo[a]pyrene	6.41	5.71	252.3	C1=CC=C2C3=C4C(=CC2=C1)C=CC5=C4C(=CC=C5)C=C3	1.14	3.07	-1.25	Tao et al., 2009	Wheat
Benzo[a]pyrene	6.41	3.47	252.3	C1=CC=C2C3=C4C(=CC2=C1)C=CC5=C4C(=CC=C5)C=C3	1.14	3.13	-0.98	Tao et al., 2009	Wheat
Benzo[a]pyrene	6.41	6.22	252.3	C1=CC=C2C3=C4C(=CC2=C1)C=CC5=C4C(=CC=C5)C=C3	1.14	3.31	-1.05	Tao et al., 2009	Wheat
Dibenzo[a,h]anthracene	6.75	4.33	278.3	C1=CC=C2C(=C1)C=CC3=CC4=C(C=CC5=CC=CC=C54)C=C32	1.14	3.12	-1.49	Tao et al., 2009	Wheat
Dibenzo[a,h]anthracene	6.75	2.71	278.3	C1=CC=C2C(=C1)C=CC3=CC4=C(C=CC5=CC=CC=C54)C=C32	1.14	3.23	-1.17	Tao et al., 2009	Wheat
Dibenzo[a,h]anthracene	6.75	2.60	278.3	C1=CC=C2C(=C1)C=CC3=CC4=C(C=CC5=CC=CC=C54)C=C32	1.14	3.00	-1.39	Tao et al., 2009	Wheat
Dibenzo[a,h]anthracene	6.75	3.47	278.3	C1=CC=C2C(=C1)C=CC3=CC4=C(C=CC5=CC=CC=C54)C=C32	1.14	3.29	-1.22	Tao et al., 2009	Wheat

Dibenzo[a,h]anthracene	6.75	5.31	278.3	C1=CC=C2C(=C1)C=CC3=CC4=C(C=CC5=CC=CC=C54)C=C32	1.14	3.15	-1.55	Tao et al., 2009	Wheat
Dibenzo[a,h]anthracene	6.75	3.47	278.3	C1=CC=C2C(=C1)C=CC3=CC4=C(C=CC5=CC=CC=C54)C=C32	1.14	3.41	-1.10	Tao et al., 2009	Wheat
Benzo[g,h,i]perylene	6.90	1.41	276.3	C1=CC2=C3C(=C1)C4=CC=CC5=C4C6=C(C=C5)C=CC(=C36)C=C2	1.14	3.06	-1.22	Tao et al., 2009	Wheat
Benzo[g,h,i]perylene	6.90	2.71	276.3	C1=CC2=C3C(=C1)C4=CC=CC5=C4C6=C(C=C5)C=CC(=C36)C=C2	1.14	3.57	-0.99	Tao et al., 2009	Wheat
Benzo[g,h,i]perylene	6.90	5.71	276.3	C1=CC2=C3C(=C1)C4=CC=CC5=C4C6=C(C=C5)C=CC(=C36)C=C2	1.14	3.62	-1.25	Tao et al., 2009	Wheat
Benzo[g,h,i]perylene	6.90	2.60	276.3	C1=CC2=C3C(=C1)C4=CC=CC5=C4C6=C(C=C5)C=CC(=C36)C=C2	1.14	3.18	-1.36	Tao et al., 2009	Wheat
Benzo[g,h,i]perylene	6.90	5.31	276.3	C1=CC2=C3C(=C1)C4=CC=CC5=C4C6=C(C=C5)C=CC(=C36)C=C2	1.14	3.20	-1.65	Tao et al., 2009	Wheat
Atrazine	2.71	3.55	215.68	CCNC1=NC(=NC(=N1)Cl)NC(C)C	1.00	0.80	0.08	Trapp et al., 1990	Barely
1,2,4-Trichlorobenzene	3.98	3.55	181.4	C1=CC(=C(C=C1Cl)Cl)Cl	1.00	1.28	0.03	Trapp et al., 1990	Barely
1,2,3,5-Tetrachlorobenzene	4.59	3.55	215.9	C1=C(C=C(C(=C1Cl)Cl)Cl)Cl	1.00	2.15	0.23	Trapp et al., 1990	Barely
Dieldrin	4.55	3.55	380.9	C1C2C3C(C1C4C2O4)C5(C(=C(C3(C5(Cl)Cl)Cl)Cl)Cl)Cl	1.00	1.98	-0.26	Trapp et al., 1990	Barely
Hexachlorobenzene	5.50	3.55	284.8	C1(=C(C(=C(C(=C1Cl)Cl)Cl)Cl)Cl)Cl	1.00	2.87	0.07	Trapp et al., 1990	Barely
2,4,6,2',4'-PCB	5.92	3.55	326.4	C1=CC(=C(C=C1Cl)C2=CC(=C(C=C2Cl)Cl)Cl)Cl	1.00	3.20	0.07	Trapp et al., 1990	Barely

DDT	6.36	3.55	354.5	C1=CC(=CC=C1C(C2=CC=C(C=C2)Cl)C(Cl)(Cl)Cl)Cl	1.00	3.41	-0.48	Trapp et al., 1990	Barely
Phenanthrene	4.46	2.00	178.23	C1=CC=C2C(=C1)C=CC3=CC=CC=C32	0.24	1.49	-0.49	Kipopoulou et al., 1999	Carrot
Anthracene	4.54	2.00	178.23	C1=CC=C2C=C3C=CC=CC3=CC2=C1	0.24	1.21	-0.85	Kipopoulou et al., 1999	Carrot
Fluoranthene	5.16	2.00	202.25	C1=CC=C2C(=C1)C3=CC=CC4=C3C2=CC=C4	0.24	1.73	-0.95	Kipopoulou et al., 1999	Carrot
Pyrene	5.18	2.00	202.25	C1=CC2=C3C(=C1)C=CC4=CC=CC(=C43)C=C2	0.24	1.85	-0.85	Kipopoulou et al., 1999	Carrot
Benzo[a]anthracene	5.61	2.00	228.3	C1=CC=C2C(=C1)C=CC3=CC4=CC=CC=C4C=C32	0.24	1.36	-1.77	Kipopoulou et al., 1999	Carrot
Chrysene	5.73	2.00	228.3	C1=CC=C2C(=C1)C=CC3=C2C=CC4=CC=CC=C43	0.24	1.62	-1.64	Kipopoulou et al., 1999	Carrot
Benzo[e]pyrene	6.44	2.00	252.3	C1=CC=C2C(=C1)C3=CC=CC4=C3C5=C(C=CC=C25)C=C4	0.24	2.22	-1.74	Kipopoulou et al., 1999	Carrot
Benzo[b]fluoranthene	5.78	2.00	252.3	C1=CC=C2C3=C4C(=CC=C3)C5=CC=CC=C5C4=CC2=C1	0.24	1.38	-1.92	Kipopoulou et al., 1999	Carrot
Benzo[k]fluoranthene	6.20	2.00	252.3	C1=CC=C2C=C3C4=CC=CC5=C4C(=CC=C5)C3=CC2=C1	0.24	1.87	-1.85	Kipopoulou et al., 1999	Carrot
Benzo[a]pyrene	6.41	2.00	252.3	C1=CC=C2C3=C4C(=CC2=C1)C=CC5=C4C(=CC=C5)C=C3	0.24	2.21	-1.72	Kipopoulou et al., 1999	Carrot
Dibenz-[a,h]anthracene	6.75	2.00	278.3	C1=CC=C2C(=C1)C=CC3=CC4=C(C=CC5=CC=CC=C54)C=C32	0.24	2.58	-1.70	Kipopoulou et al., 1999	Carrot
Benz[phi]perylene	6.90	2.00	276.3	C1=CC2=C3C(=C1)C4=CC=CC5=C4C6=C(C=C5)C=CC(=C36)C=C2	0.24	2.54	-1.89	Kipopoulou et al., 1999	Carrot

Indeno[1,2,3-cd]pyrene	6.70	2.00	276.3	C1=CC=C2C(=C1)C3=C4C2=CC5=CC=CC6=C5C4=C(C=C6)C=C3	0.24	2.43	-1.80	Kipopoulou et al., 1999	Carrot
Galaxolide	5.90	1.55	258.4	CC1COCC2=CC3=C(C=C12)C(C(C3(C)C)C)(C)C	0.24	1.69	-1.05	Macherius et al., 2012	Carrot
Galaxolide	5.90	1.55	258.4	CC1COCC2=CC3=C(C=C12)C(C(C3(C)C)C)(C)C	1.00	1.66	-1.08	Macherius et al., 2012	Barely
Tonalide	5.70	1.55	258.4	Cc1cc2c(cc1C(C)=O)C(C)(C)CC(C)C2(C)C	0.24	1.26	-1.30	Macherius et al., 2012	Carrot
Tonalide	5.70	1.55	258.4	Cc1cc2c(cc1C(C)=O)C(C)(C)CC(C)C2(C)C	1.00	1.74	-0.83	Macherius et al., 2012	Barely
Triclocarban	4.90	3.80	315.6	C1=CC(=CC=C1NC(=O)NC2=CC(=C(C=C2)Cl)Cl)Cl	0.10	0.91	-1.51	Wu et al., 2012	Radish
Triclosan	4.80	13.80	289.5	C1=CC(=C(C=C1Cl)O)OC2=C(C=C(C=C2)Cl)Cl	0.10	1.41	-1.03	Pannu et al., 2012	Radish
Triclosan	4.80	4.10	289.5	C1=CC(=C(C=C1Cl)O)OC2=C(C=C(C=C2)Cl)Cl	0.10	1.04	-0.80	Prosser et al., 2014	Radish
Triclosan	4.80	3.90	289.5	C1=CC(=C(C=C1Cl)O)OC2=C(C=C(C=C2)Cl)Cl	0.24	1.27	-0.62	Prosser et al., 2014	Carrot
Trimethoprim	0.91	0.69	290.32	COC1=CC(=CC(=C1OC)OC)CC2=CN=C(N=C2N)N	0.24	-0.07	-1.10	Boxall et al., 2006	Carrot
Carbamazepine	2.45	1.72	236.27	C1=CC=C2C(=C1)C=CC3=CC=CC=C3N2C(=O)N	0.10	0.02	0.92	Carter et al., 2014	Radish
BDE-66	6.29	1.90	485.79	C1=CC(=C(C=C1OC2=C(C=C(C=C2)Br)Br)Br)Br	0.70		-1.19	Huang et al., 2011	Pumpkin
BDE-66	6.29	1.90	485.79	C1=CC(=C(C=C1OC2=C(C=C(C=C2)Br)Br)Br)Br	0.53		-1.28	Huang et al., 2011	Maize
BDE-66	6.29	1.90	485.79	C1=CC(=C(C=C1OC2=C(C=C(C=C2)Br)Br)Br)Br	0.56		-1.24	Huang et al., 2011	Ryegrass

BDE-66	6.29	3.19	485.79	C1=CC(=C(C=C1OC2=C(C=C(C=C2)Br)Br)Br)Br	0.70	-0.93	Huang et al., 2011	Pumpkin
BDE-66	6.29	3.19	485.79	C1=CC(=C(C=C1OC2=C(C=C(C=C2)Br)Br)Br)Br	0.53	-0.84	Huang et al., 2011	Maize
BDE-66	6.29	3.19	485.79	C1=CC(=C(C=C1OC2=C(C=C(C=C2)Br)Br)Br)Br	0.56	-0.95	Huang et al., 2011	Ryegrass
BDE-66	6.29	0.98	485.79	C1=CC(=C(C=C1OC2=C(C=C(C=C2)Br)Br)Br)Br	0.70	-2.08	Huang et al., 2011	Pumpkin
BDE-66	6.29	0.98	485.79	C1=CC(=C(C=C1OC2=C(C=C(C=C2)Br)Br)Br)Br	0.53	-1.77	Huang et al., 2011	Maize
BDE-66	6.29	0.98	485.79	C1=CC(=C(C=C1OC2=C(C=C(C=C2)Br)Br)Br)Br	0.56	-1.72	Huang et al., 2011	Ryegrass
BDE-85	6.69	1.90	564.7	C1=CC(=C(C=C1Br)Br)OC2=C(C(=C(C=C2)Br)Br)Br	0.70	-1.43	Huang et al., 2011	Pumpkin
BDE-85	6.69	1.90	564.7	C1=CC(=C(C=C1Br)Br)OC2=C(C(=C(C=C2)Br)Br)Br	0.53	-1.40	Huang et al., 2011	Maize
BDE-85	6.69	1.90	564.7	C1=CC(=C(C=C1Br)Br)OC2=C(C(=C(C=C2)Br)Br)Br	0.56	-1.33	Huang et al., 2011	Ryegrass
BDE-85	6.69	3.19	564.7	C1=CC(=C(C=C1Br)Br)OC2=C(C(=C(C=C2)Br)Br)Br	0.70	-1.17	Huang et al., 2011	Pumpkin
BDE-85	6.69	3.19	564.7	C1=CC(=C(C=C1Br)Br)OC2=C(C(=C(C=C2)Br)Br)Br	0.53	-1.01	Huang et al., 2011	Maize
BDE-85	6.69	3.19	564.7	C1=CC(=C(C=C1Br)Br)OC2=C(C(=C(C=C2)Br)Br)Br	0.56	-1.24	Huang et al., 2011	Ryegrass
BDE-85	6.69	0.98	564.7	C1=CC(=C(C=C1Br)Br)OC2=C(C(=C(C=C2)Br)Br)Br	0.70	-1.14	Huang et al., 2011	Pumpkin
BDE-85	6.69	0.98	564.7	C1=CC(=C(C=C1Br)Br)OC2=C(C(=C(C=C2)Br)Br)Br	0.53	-1.10	Huang et al., 2011	Maize

BDE-85	6.69	0.98	564.7	C1=CC(=C(C=C1Br)Br)OC2=C(C(=C(C=C2)Br)Br)Br	0.56	-1.06	Huang et al., 2011	Ryegrass
BDE-191	7.49	3.19	722.5	C1=C(C=C(C(=C1Br)Br)Br)OC2=C(C(=C(C=C2Br)Br)Br)Br	0.70	-1.05	Huang et al., 2011	Pumpkin
BDE-191	7.49	3.19	722.5	C1=C(C=C(C(=C1Br)Br)Br)OC2=C(C(=C(C=C2Br)Br)Br)Br	0.53	-0.82	Huang et al., 2011	Maize
BDE-191	7.49	3.19	722.5	C1=C(C=C(C(=C1Br)Br)Br)OC2=C(C(=C(C=C2Br)Br)Br)Br	0.56	-0.91	Huang et al., 2011	Ryegrass
BDE-191	7.49	1.90	722.5	C1=C(C=C(C(=C1Br)Br)Br)OC2=C(C(=C(C=C2Br)Br)Br)Br	0.70	-0.83	Huang et al., 2011	Pumpkin
BDE-191	7.49	1.90	722.5	C1=C(C=C(C(=C1Br)Br)Br)OC2=C(C(=C(C=C2Br)Br)Br)Br	0.53	-0.85	Huang et al., 2011	Maize
BDE-191	7.49	1.90	722.5	C1=C(C=C(C(=C1Br)Br)Br)OC2=C(C(=C(C=C2Br)Br)Br)Br	0.56	-1.06	Huang et al., 2011	Ryegrass
BDE-191	7.49	0.98	722.5	C1=C(C=C(C(=C1Br)Br)Br)OC2=C(C(=C(C=C2Br)Br)Br)Br	0.70	-1.44	Huang et al., 2011	Pumpkin
BDE-191	7.49	0.98	722.5	C1=C(C=C(C(=C1Br)Br)Br)OC2=C(C(=C(C=C2Br)Br)Br)Br	0.53	-1.04	Huang et al., 2011	Maize
BDE-191	7.49	0.98	722.5	C1=C(C=C(C(=C1Br)Br)Br)OC2=C(C(=C(C=C2Br)Br)Br)Br	0.56	-1.20	Huang et al., 2011	Ryegrass
BDE-197	7.90	3.19	801.4	C1=C(C(=C(C(=C1Br)Br)Br)OC2=C(C(=C(C=C2Br)Br)Br)Br)Br	0.70	-1.43	Huang et al., 2011	Pumpkin
BDE-197	7.90	3.19	801.4	C1=C(C(=C(C(=C1Br)Br)Br)OC2=C(C(=C(C=C2Br)Br)Br)Br)Br	0.53	-1.38	Huang et al., 2011	Maize
BDE-197	7.90	3.19	801.4	C1=C(C(=C(C(=C1Br)Br)Br)OC2=C(C(=C(C=C2Br)Br)Br)Br)Br	0.56	-1.19	Huang et al., 2011	Ryegrass
BDE-197	7.90	1.90	801.4	C1=C(C(=C(C(=C1Br)Br)Br)OC2=C(C(=C(C=C2Br)Br)Br)Br)Br	0.70	-1.08	Huang et al., 2011	Pumpkin

BDE-197	7.90	1.90	801.4	C1=C(C(=C(C(=C1Br)Br)Br)OC2=C(C(=C(C=C2Br)Br)Br)Br)Br	0.53	-1.18	Huang et al., 2011	Maize
BDE-197	7.90	1.90	801.4	C1=C(C(=C(C(=C1Br)Br)Br)OC2=C(C(=C(C=C2Br)Br)Br)Br)Br	0.56	-1.49	Huang et al., 2011	Ryegrass
BDE-197	7.90	0.98	801.4	C1=C(C(=C(C(=C1Br)Br)Br)OC2=C(C(=C(C=C2Br)Br)Br)Br)Br	0.70	-1.32	Huang et al., 2011	Pumpkin
BDE-197	7.90	0.98	801.4	C1=C(C(=C(C(=C1Br)Br)Br)OC2=C(C(=C(C=C2Br)Br)Br)Br)Br	0.53	-1.42	Huang et al., 2011	Maize
BDE-197	7.90	0.98	801.4	C1=C(C(=C(C(=C1Br)Br)Br)OC2=C(C(=C(C=C2Br)Br)Br)Br)Br	0.56	-1.68	Huang et al., 2011	Ryegrass
BDE-208	8.30	3.19	880.3	C1=C(C(=C(C(=C1Br)Br)OC2=C(C(=C(C(=C2Br)Br)Br)Br)Br)Br)Br	0.70	-2.02	Huang et al., 2011	Pumpkin
BDE-208	8.30	1.90	880.3	C1=C(C(=C(C(=C1Br)Br)OC2=C(C(=C(C(=C2Br)Br)Br)Br)Br)Br)Br	0.70	-2.16	Huang et al., 2011	Pumpkin
BDE-208	8.30	1.90	880.3	C1=C(C(=C(C(=C1Br)Br)OC2=C(C(=C(C(=C2Br)Br)Br)Br)Br)Br)Br	0.53	-2.13	Huang et al., 2011	Maize
BDE-208	8.30	1.90	880.3	C1=C(C(=C(C(=C1Br)Br)OC2=C(C(=C(C(=C2Br)Br)Br)Br)Br)Br)Br	0.56	-2.34	Huang et al., 2011	Ryegrass
BDE-208	8.30	0.98	880.3	C1=C(C(=C(C(=C1Br)Br)OC2=C(C(=C(C(=C2Br)Br)Br)Br)Br)Br)Br	0.70	-2.30	Huang et al., 2011	Pumpkin
BDE-208	8.30	0.98	880.3	C1=C(C(=C(C(=C1Br)Br)OC2=C(C(=C(C(=C2Br)Br)Br)Br)Br)Br)Br	0.53	-2.30	Huang et al., 2011	Maize
BDE-208	8.30	0.98	880.3	C1=C(C(=C(C(=C1Br)Br)OC2=C(C(=C(C(=C2Br)Br)Br)Br)Br)Br)Br	0.56	-2.40	Huang et al., 2011	Ryegrass
BDE-207	8.30	3.19	880.3	C1=C(C(=C(C(=C1Br)Br)Br)OC2=C(C(=C(C(=C2Br)Br)Br)Br)Br)Br	0.70	-1.26	Huang et al., 2011	Pumpkin
BDE-207	8.30	3.19	880.3	C1=C(C(=C(C(=C1Br)Br)Br)OC2=C(C(=C(C(=C2Br)Br)Br)Br)Br)Br	0.53	-1.49	Huang et al., 2011	Maize

BDE-207	8.30	3.19	880.3	C1=C(C(=C(C(=C1Br)Br)Br)OC2=C(C(=C(C(=C2Br)Br)Br)Br)Br)Br	0.56	-1.60	Huang et al., 2011	Ryegrass
BDE-207	8.30	1.90	880.3	C1=C(C(=C(C(=C1Br)Br)Br)OC2=C(C(=C(C(=C2Br)Br)Br)Br)Br)Br	0.70	-2.60	Huang et al., 2011	Pumpkin
BDE-207	8.30	1.90	880.3	C1=C(C(=C(C(=C1Br)Br)Br)OC2=C(C(=C(C(=C2Br)Br)Br)Br)Br)Br	0.53	-2.15	Huang et al., 2011	Maize
BDE-207	8.30	1.90	880.3	C1=C(C(=C(C(=C1Br)Br)Br)OC2=C(C(=C(C(=C2Br)Br)Br)Br)Br)Br	0.56	-2.45	Huang et al., 2011	Ryegrass
BDE-207	8.30	0.98	880.3	C1=C(C(=C(C(=C1Br)Br)Br)OC2=C(C(=C(C(=C2Br)Br)Br)Br)Br)Br	0.70	-2.01	Huang et al., 2011	Pumpkin
BDE-207	8.30	0.98	880.3	C1=C(C(=C(C(=C1Br)Br)Br)OC2=C(C(=C(C(=C2Br)Br)Br)Br)Br)Br	0.53	-1.74	Huang et al., 2011	Maize
BDE-207	8.30	0.98	880.3	C1=C(C(=C(C(=C1Br)Br)Br)OC2=C(C(=C(C(=C2Br)Br)Br)Br)Br)Br	0.56	-1.92	Huang et al., 2011	Ryegrass
alpha-endosulfan	0.50	8.80	406.9	C1[C@@H]2[C@H](COS(=O)O1)[C@]3(C(=C([C@@]2(C3(Cl)Cl)Cl)Cl)Cl)Cl	0.10	-0.61	GONZALEZ et al., 2003	leek
endosulfan sulfate	0.56	8.80	422.9	C1C2C(COS(=O)(=O)O1)C3(C(=C(C2(C3(Cl)Cl)Cl)Cl)Cl)Cl	0.10	0.38	GONZALEZ et al., 2003	leek
dieldrin	0.72	8.80	380.9	C1C2C3C(C1C4C2O4)C5(C(=C(C3(C5(Cl)Cl)Cl)Cl)Cl)Cl	0.10	-0.66	GONZALEZ et al., 2003	leek
heptachlor	0.72	8.80	373.3	C1=CC(C2C1C3(C(=C(C2(C3(Cl)Cl)Cl)Cl)Cl)Cl)Cl	0.10	0.22	GONZALEZ et al., 2003	leek
heptachlor epoxide	0.62	8.80	389.3	C12C(C(C3C1O3)Cl)C4(C(=C(C2(C4(Cl)Cl)Cl)Cl)Cl)Cl	0.10	-0.87	GONZALEZ et al., 2003	leek
Imidacloprid	0.57	3.05	255.66	C1CN(C(=N[N+](=O)[O-])N1)CC2=CN=C(C=C2)Cl	0.53	-0.31	Wang et.al., 2020	Maize
Acetamiprid	0.80	3.05	222.67	CC(=NC#N)N(C)CC1=CN=C(C=C1)Cl	0.53	-0.18	Wang et.al., 2020	Maize
Tricyclazole	1.70	3.05	189.24	CC1=C2C(=CC=C1)SC3=NN=CN23	0.53	-0.24	Wang et.al., 2020	Maize

Azoxystrobin	2.50	3.05	403.4	COC=C(C1=CC=CC=C1OC2=NC=NC(=C2)OC3=CC=CC=C3C#N)C(=O)OC	0.53	-0.14	Wang et.al., 2020	Maize
Tebuconazole	3.70	3.05	307.82	CC(C)(C)C(CCC1=CC=C(C=C1)Cl)(CN2C=NC=N2)O	0.53	-0.08	Wang et.al., 2020	Maize
Difenoconazole	4.40	3.05	406.3	CC1COC(O1)(CN2C=NC=N2)C3=C(C=C(C=C3)OC4=CC=C(C=C4)Cl)Cl	0.53	-0.57	Wang et.al., 2020	Maize

Table S4: Parameters tuned with five-fold cross validation in GBRT model.

N_estimators	100, 200, 250, 500, 750, 1000
Max depth	2, 3, 4, 5, 6

Pseudocode for model 5-fold cross validation:

Define sets of model hyperparameters P for evaluation

Divide data into K = 5 equal folds

For fold i in the K folds:

    Set fold i as test set

    Perform feature selection based on remaining 4 folds

For parameter combination p from P:

Set 12.5% of the data from remaining 4 folds as validation set (10% of overall dataset)

Train model on the left 87.5% of data from remaining 4 folds

Evaluate model performance on validation set

if model has better performance on validation set:

Evaluate and update model performance on test set

Calculate the average performance on K=5 folds