**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.



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-17BDE-183BDE-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 xi and target yi, the model calculates:

$\hat{y\_{i}}$ = $F\_{M}\left(x\_{i}\right)$= $\sum\_{m=1}^{M}h\_{m}\left(xi\right)$

Here $h\_{m}$ are the weak learners, which are decision trees in this study. $\hat{y\_{i}}$ are the predicted values through the model.

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

$F\_{M}\left(x\_{i}\right)$= $F\_{M-1}\left(x\_{i}\right)+h\_{m}\left(x\right)$

where the newly added tree $h\_{m}\left(x\right)$ is fitted in order to minimize a sum of *loss* given the previous ensemble $F\_{M-1}$:

$$h\_{m}=argminL\_{m}=argmin\sum\_{i=1}^{n}loss\left(y\_{i},F\_{M-1}\left(x\_{i}\right)+h\left(x\_{i}\right)\right)$$

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)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)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)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)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)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)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)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)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)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)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)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 |