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.

![Chemical structures](image)

**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, Azoxytrobin |

### 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:

$$\hat{y}_i = F_M(x_i) = \sum_{m=1}^{M} h_m(x_i)$$

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:

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

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

$$h_m = \arg\min L_m = \arg\min \sum_{i=1}^{n} loss(y_i, F_{M-1}(x_i) + h(x_i))$$

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 on the predicted outcome of a machine learning model. The influences of changes of $\log K_{ow}$, $f_{om}$, $f_{lipid}$ 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) $\log K_{ow}$; (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=C(2)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=C(2)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=C(2)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=C(2)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=C(2)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(C1Cl)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(C1Cl)Cl)Cl)Cl)Cl | 0.24     | 1.35          | -2.92        | Harris and Sans, 1967  | Carrot |
| Dieldrin   | 4.55    | 1.40    | 380.9  | C1C2C3(C1C4C2O4)C5(C=C(C3(C5(C1Cl)Cl)Cl)Cl)Cl | 0.24     | 1.23          | -0.60        | Harris and Sans, 1967  | Carrot |
| Dieldrin   | 4.55    | 3.60    | 380.9  | C1C2C3(C1C4C2O4)C5(C=C(C3(C5(C1Cl)Cl)Cl)Cl)Cl | 0.24     | 1.25          | -0.99        | Harris and Sans, 1967  | Carrot |
| Dieldrin   | 4.55    | 66.50   | 380.9  | C1C2C3(C1C4C2O4)C5(C=C(C3(C5(C1Cl)Cl)Cl)Cl)Cl | 0.24     | 1.22          | -2.29        | Harris and Sans, 1967  | Carrot |
| Dieldrin   | 4.55    | 3.60    | 380.9  | C1C2C3(C1C4C2O4)C5(C=C(C3(C5(C1Cl)Cl)Cl)Cl)Cl | 0.10     | 0.91          | -1.33        | Harris and Sans, 1967  | Radish|
| Dieldrin   | 4.55    | 66.50   | 380.9  | C1C2C3(C1C4C2O4)C5(C=C(C3(C5(C1Cl)Cl)Cl)Cl)Cl | 0.10     | 0.92          | -2.59        | Harris and Sans, 1967  | Radish|
| Compound   | 4.55  | 3.60  | 380.9 | C1C2C3C(C1C4C2O4)C5(C(=C(C3(C5( | 0.10  | 0.69  | -1.56 | Harris and Sans, 1967 | Turnips |
|------------|-------|-------|-------|-----------------|-------|-------|-------|---------------------|-------|
| m-DCB (1,3-DCB) | 3.44  | 2.82  | 147   | C1=CC(=C(C=C1Cl)Cl | 0.34  | 1.00  | 0.22  | Zhang et al., 2005 | Spinach |
| m-DCB (1,3-DCB) | 3.44  | 0.78  | 147   | C1=CC(=C(C=C1Cl)Cl | 0.34  | 0.83  | 0.61  | Zhang et al., 2005 | Spinach |
| m-DCB (1,3-DCB) | 3.44  | 1.41  | 147   | C1=CC(=C(C=C1Cl)Cl | 0.24  | 0.45  | -0.03 | Zhang et al., 2005 | Carrot |
| m-DCB (1,3-DCB) | 3.44  | 0.78  | 147   | C1=CC(=C(C=C1Cl)Cl | 0.24  | 0.11  | -0.12 | Zhang et al., 2005 | Carrot |
| m-DCB (1,3-DCB) | 3.44  | 2.82  | 147   | C1=CC(=C(C=C1Cl)Cl | 0.09  | 0.19  | -0.59 | Zhang et al., 2005 | Radish |
| m-DCB (1,3-DCB) | 3.44  | 0.78  | 147   | C1=CC(=C(C=C1Cl)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=C1Cl)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=C1Cl)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=C1Cl)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 | 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 | 0.34  | 0.90  | -0.10 | Zhang et al., 2005 | Spinach |
| Compound                  | LogP  | MW    | Molecular Structure                                      | pIC50 | pIC50 | pIC50 | Ref          | Plant Type |
|---------------------------|-------|-------|----------------------------------------------------------|-------|-------|-------|--------------|------------|
| 1,2,4-TCB                 | 4.02  | 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  | 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  | 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  | 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  | 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  | 181.4 | C1=CC(=C(C=C1Cl)Cl)Cl                                    | 0.09  | 0.24  | -0.76 | Zhang et al., 2005 | Radish     |
| Fluorene                  | 4.18  | 166.22| C1C2=CC=CC=C2C3=CC=CC=C31                                 | 0.10  | 0.92  | -1.59 | Cai et al., 2008 | Radish     |
| Phenanthrene              | 4.46  | 178.23| C1=CC=C2C(=C1)C=C3=C3=CC=CC=C3                            | 0.10  | 1.34  | -1.45 | Cai et al., 2008 | Radish     |
| Phenanthrene              | 4.46  | 178.23| C1=CC=C2C(=C1)C=C3=C3=CC=CC=C3                            | 0.10  | 1.32  | -1.05 | Cai et al., 2008 | Radish     |
| Anthracene                | 4.54  | 178.23| C1=CC=C2C=C3C=CC=CC3=C3=C2=C1                             | 0.10  | 0.71  | -1.63 | Cai et al., 2008 | Radish     |
| Anthracene                | 4.54  | 178.23| C1=CC=C2C=C3C=CC=CC3=C3=C2=C1                             | 0.10  | 0.71  | -2.15 | Cai et al., 2008 | Radish     |
| Fluoranthene              | 5.16  | 202.25| C1=CC=C2C(=C1)C=C3=C3=CC=C3                              | 0.10  | 1.56  | -0.72 | Cai et al., 2008 | Radish     |
| Benzo[a]pyrene            | 6.34  | 252.3 | C1=CC=C2C3=C4C(=CC2=C1)C=CC5=C4(=CC=C5)C=C3              | 0.10  | 1.62  | -2.52 | Cai et al., 2008 | Radish     |
| Di(2-ethylhexyl) phthalate| 7.60  | 390.6 | CCCCC(CCC)COC(=O)C1=CC=CC=C1C(=O)OCC(CCC)CCCC             | 0.10  | 2.80  | -1.94 | Cai et al., 2008 | Radish     |
| Di(2-ethylhexyl) phthalate| 7.60  | 390.6 | CCCCC(CCC)COC(=O)C1=CC=CC=C1C(=O)OCC(CCC)CCCC             | 0.10  | 2.98  | -2.40 | Cai et al., 2008 | Radish     |
| Phenanthrene              | 4.46  | 178.23| C1=CC=C2C(=C1)C=C3=C3=CC=CC=C3                            | 0.32  | 0.57  | -1.27 | Gao et al., 2005 | Ryegrass   |

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| Substance   | Concentration | Temperature | LogKow | LogP | Ref.          | Plant          |
|-------------|---------------|-------------|--------|------|--------------|----------------|
| Phenanthrene| 4.46          | 1.45        | 178.23 | 0.68 | Gao et al., 2005 | Chinese cabbage|
| Phenanthrene| 4.46          | 1.45        | 178.23 | 0.32 | Gao et al., 2005 | Amaranth      |
| Pyrene      | 5.18          | 1.45        | 202.25 | 0.32 | Gao et al., 2005 | Ryegrass      |
| Pyrene      | 5.18          | 1.45        | 202.25 | 0.68 | Gao et al., 2005 | Chinese cabbage|
| alpha-HCH   | 3.81          | 6.36        | 290.83 | 0.10 | Mikes et al., 2009 | Radish        |
| HCB         | 5.50          | 6.36        | 284.8  | 0.10 | Mikes et al., 2009 | Radish        |
| o,p'-DDE    | 5.76          | 6.36        | 318    | 0.10 | Mikes et al., 2009 | Radish        |
| p,p'-DDE    | 5.91          | 6.36        | 318    | 0.10 | Mikes et al., 2009 | Radish        |
| o,p'-DDD    | 5.82          | 6.36        | 320    | 0.10 | Mikes et al., 2009 | Radish        |
| p,p'-DDD    | 5.69          | 6.36        | 320    | 0.10 | Mikes et al., 2009 | Radish        |
| o,p'-DDT    | 6.19          | 6.36        | 354.5  | 0.10 | Mikes et al., 2009 | Radish        |
| p,p'-DDT    | 5.98          | 6.36        | 354.5  | 0.10 | Mikes et al., 2009 | Radish        |
| PCB 101     | 6.50          | 6.36        | 326.4  | 0.10 | Mikes et al., 2009 | Radish        |
| PCB 153     | 6.90          | 6.36        | 360.9  | 0.10 | Mikes et al., 2009 | Radish        |
| PCB 138     | 6.69          | 6.36        | 360.9  | 0.10 | Mikes et al., 2009 | Radish        |
| Compound | BDE | pIC50 | logKow | BDE | pIC50 | logKow |
|----------|-----|-------|--------|-----|-------|--------|
| PCB 180  | 7.20| 6.36  | 395.3  | 0.10| 2.40  | -2.07  |
| BDE-100  | 7.24| 3.19  | 564.7  | 0.53| 2.61  | -1.66  |
| BDE-100  | 7.24| 3.19  | 564.7  | 0.56| 2.76  | -1.51  |
| BDE-100  | 7.24| 1.90  | 564.7  | 0.70| 2.88  | -1.17  |
| BDE-100  | 7.24| 1.90  | 564.7  | 0.53| 2.84  | -1.21  |
| BDE-100  | 7.24| 1.90  | 564.7  | 0.56| 2.67  | -1.37  |
| BDE-100  | 7.24| 0.98  | 564.7  | 0.70| 2.69  | -1.07  |
| BDE-100  | 7.24| 0.98  | 564.7  | 0.53| 2.70  | -1.05  |
| BDE-100  | 7.24| 0.98  | 564.7  | 0.56| 2.84  | -0.92  |
| BDE-153  | 7.90| 3.19  | 643.6  | 0.70| 2.95  | -1.92  |
| BDE-153  | 7.90| 3.19  | 643.6  | 0.56| 3.64  | -1.23  |
| BDE-153  | 7.90| 1.90  | 643.6  | 0.70| 3.19  | -1.45  |
| BDE-153  | 7.90| 1.90  | 643.6  | 0.53| 3.39  | -1.25  |
| BDE-153  | 7.90| 1.90  | 643.6  | 0.56| 3.37  | -1.27  |
| Compound | BDE | DTE | DP | Structure | Log Kow | Log P | log D | Huang et al., 2011 | Plant Type |
|----------|-----|-----|----|-----------|--------|------|------|-------------------|------------|
| 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 | 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 | 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 | Ryegrass |
| BDE-154  | 7.82| 3.19| 643.6| C1=C(C=C(C(=C1Br)Br)Br)OC2=CC(=C(C=C2Br)Br)Br | 0.70 | 3.52 | -1.27 | Pumpkin |
| BDE-154  | 7.82| 3.19| 643.6| C1=C(C=C(C(=C1Br)Br)Br)OC2=CC(=C(C=C2Br)Br)Br | 0.53 | 3.59 | -1.20 | Maize |
| BDE-154  | 7.82| 1.90| 643.6| C1=C(C=C(C(=C1Br)Br)Br)OC2=CC(=C(C=C2Br)Br)Br | 0.70 | 3.34 | -1.23 | Pumpkin |
| BDE-154  | 7.82| 1.90| 643.6| C1=C(C=C(C(=C1Br)Br)Br)OC2=CC(=C(C=C2Br)Br)Br | 0.53 | 3.24 | -1.33 | Maize |
| BDE-154  | 7.82| 1.90| 643.6| C1=C(C=C(C(=C1Br)Br)Br)OC2=CC(=C(C=C2Br)Br)Br | 0.56 | 3.16 | -1.41 | Ryegrass |
| BDE-154  | 7.82| 0.98| 643.6| C1=C(C=C(C(=C1Br)Br)Br)OC2=CC(=C(C=C2Br)Br)Br | 0.70 | 3.14 | -1.15 | Pumpkin |
| BDE-154  | 7.82| 0.98| 643.6| C1=C(C=C(C(=C1Br)Br)Br)OC2=CC(=C(C=C2Br)Br)Br | 0.53 | 3.22 | -1.06 | Maize |
| BDE-154  | 7.82| 0.98| 643.6| C1=C(C=C(C(=C1Br)Br)Br)OC2=CC(=C(C=C2Br)Br)Br | 0.56 | 3.14 | -1.14 | 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 | 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 | 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 | Ryegrass |
| Compound | Molecular Weight | LogP | Notes |
|----------|------------------|------|-------|
| BDE-17   | 5.74             | 1.90 |       |
|          | 406.89           |      | Huang et al., 2011 Pumpkin |
| BDE-17   | 5.74             | 1.90 |       |
|          | 406.89           |      | Huang et al., 2011 Maize   |
| BDE-17   | 5.74             | 1.90 |       |
|          | 406.89           |      | Huang et al., 2011 Ryegrass |
| BDE-17   | 5.74             | 0.98 |       |
|          | 406.89           |      | Huang et al., 2011 Pumpkin |
| BDE-183  | 8.27             | 3.19 |       |
|          | 722.5            |      | Huang et al., 2011 Pumpkin |
| BDE-183  | 8.27             | 3.19 |       |
|          | 722.5            |      | Huang et al., 2011 Maize   |
| BDE-183  | 8.27             | 3.19 |       |
|          | 722.5            |      | Huang et al., 2011 Ryegrass |
| BDE-183  | 8.27             | 1.90 |       |
|          | 722.5            |      | Huang et al., 2011 Pumpkin |
| BDE-183  | 8.27             | 1.90 |       |
|          | 722.5            |      | Huang et al., 2011 Maize   |
| BDE-183  | 8.27             | 0.98 |       |
|          | 722.5            |      | Huang et al., 2011 Pumpkin |
| BDE-183  | 8.27             | 0.98 |       |
|          | 722.5            |      | Huang et al., 2011 Maize   |
| BDE-183  | 8.27             | 0.98 |       |
|          | 722.5            |      | Huang et al., 2011 Ryegrass |
| BDE-206  | 8.47             | 3.19 |       |
|          | 880.3            |      | Huang et al., 2011 Pumpkin |
| Compound | Mulliken Charge | Delta Mulliken Charge | Log P | Source | Plant |
|----------|----------------|-----------------------|-------|--------|-------|
| BDE-206  | 8.47           | 3.19                  | 880.3 | 0.53   | 4.43  | -0.95 | Huang et al., 2011 | Maize |
| BDE-206  | 8.47           | 3.19                  | 880.3 | 0.56   | 3.78  | -1.60 | Huang et al., 2011 | Ryegrass |
| BDE-206  | 8.47           | 1.90                  | 880.3 | 0.70   | 3.13  | -1.74 | Huang et al., 2011 | Pumpkin |
| BDE-206  | 8.47           | 1.90                  | 880.3 | 0.53   | 3.37  | -1.50 | Huang et al., 2011 | Maize |
| BDE-206  | 8.47           | 1.90                  | 880.3 | 0.56   | 3.18  | -1.69 | Huang et al., 2011 | Ryegrass |
| BDE-209  | 8.70           | 0.98                  | 959.2 | 0.70   | 4.31  | -1.28 | Huang et al., 2011 | Pumpkin |
| BDE-209  | 8.70           | 3.19                  | 959.2 | 0.53   | 4.11  | -1.48 | Huang et al., 2011 | Maize |
| BDE-209  | 8.70           | 3.19                  | 959.2 | 0.56   | 4.21  | -1.38 | Huang et al., 2011 | Ryegrass |
| BDE-209  | 8.70           | 1.90                  | 959.2 | 0.70   | 3.86  | -1.50 | Huang et al., 2011 | Pumpkin |
| BDE-209  | 8.70           | 1.90                  | 959.2 | 0.53   | 3.82  | -1.54 | Huang et al., 2011 | Maize |
| BDE-209  | 8.70           | 1.90                  | 959.2 | 0.56   | 3.72  | -1.64 | Huang et al., 2011 | Ryegrass |
| BDE-28   | 5.94           | 3.19                  | 406.89| 0.53   | 1.96  | -1.13 | Huang et al., 2011 | Maize |
| BDE-28   | 5.94           | 1.90                  | 406.89| 0.53   | 1.95  | -0.92 | Huang et al., 2011 | Maize |
| BDE-28   | 5.94           | 1.90                  | 406.89| 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=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=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=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=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=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=C2Br)Br)Br | 0.56     | 2.85     | -1.27    | Huang et al., 2011 | Ryegrass|
| Compound     | m/z | Retention Time | Mass | Name                                      | Purity | Solvent | Source                  | Species |
|--------------|-----|----------------|------|-------------------------------------------|--------|---------|-------------------------|---------|
| 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                   | 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                   | 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                   | 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)| 1.10   | 1.74    | -0.61                   | 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                   | 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                    | 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                    | 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                   | 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                    | 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                   | Maize   |
| 1,4-DCB      | 3.37| 3.55           | 147  | C1=CC(=CC=C1Cl)Cl                           | 1.00   | 1.72    | 1.03                    | Barely  |
| 1,2,4-TCB    | 4.02| 3.55           | 181.4| C1=CC(=C(C=C1Cl)Cl)Cl                       | 1.00   | 1.98    | 0.65                    | Barely  |
| 1,2,3,5-TeCB | 4.59| 3.55           | 215.9| C1=C(C=C(C=C1Cl)Cl)Cl                       | 1.00   | 2.39    | 0.75                    | Barely  |
| Compound                | 5.03 | 3.55 | 250.3 | C1=C(C(=C(C1Cl)Cl)Cl)Cl | 1.00 | 2.07 | 0.03 | Scheunert et al., 1994 | Barely               |
|-------------------------|------|------|-------|--------------------------|------|------|------|------------------------|----------------------|
| Hexachlorobenzene       | 5.50 | 3.55 | 284.8 | C1=C(C(=C(C1Cl)Cl)Cl)Cl | 1.00 | 2.27 | -0.09| Scheunert et al., 1994 | Barely               |
| Naphthalene             | 3.36 | 5.31 | 128.17| C1=CC=C2C=CC2=C1         | 1.14 | 0.88 | -0.42| Tao et al., 2009       | Wheat                |
| Naphthalene             | 3.36 | 1.41 | 128.17| C1=CC=C2C=CC=C2=C1       | 1.14 | 0.72 | -0.01| Tao et al., 2009       | Wheat                |
| Naphthalene             | 3.36 | 4.33 | 128.17| C1=CC=C2C=CC=C2=C1       | 1.14 | 1.06 | -0.16| Tao et al., 2009       | Wheat                |
| Naphthalene             | 3.36 | 2.71 | 128.17| C1=CC=C2C=CC=C2=C1       | 1.14 | 1.18 | 0.17 | Tao et al., 2009       | Wheat                |
| Naphthalene             | 3.36 | 5.71 | 128.17| C1=CC=C2C=CC=C2=C1       | 1.14 | 0.73 | -0.61| Tao et al., 2009       | Wheat                |
| Naphthalene             | 3.36 | 2.60 | 128.17| C1=CC=C2C=CC=C2=C1       | 1.14 | 0.98 | -0.02| Tao et al., 2009       | Wheat                |
| Naphthalene             | 3.36 | 4.81 | 128.17| C1=CC=C2C=CC=C2=C1       | 1.14 | 0.82 | -0.44| Tao et al., 2009       | Wheat                |
| Naphthalene             | 3.36 | 2.67 | 128.17| C1=CC=C2C=CC=C2=C1       | 1.14 | 0.84 | -0.17| Tao et al., 2009       | Wheat                |
| Naphthalene             | 3.36 | 4.74 | 128.17| C1=CC=C2C=CC=C2=C1       | 1.14 | 1.08 | -0.18| Tao et al., 2009       | Wheat                |
| Naphthalene             | 3.36 | 4.16 | 128.17| C1=CC=C2C=CC=C2=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                |

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| Compound   | Mean | Median | Weight | Molecular Formula | Octanol/Water | Soil/Water | Source       | Crop  |
|------------|------|--------|--------|-------------------|---------------|-------------|--------------|-------|
| 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=C3 | 1.14          | 1.51        | -0.04        | Tao et al., 2009 | Wheat |
| Fluorene   | 4.18 | 4.33   | 166.22 | C1C2=CC=CC=C2C3=CC=CC=C3 | 1.14          | 1.76        | -0.28        | Tao et al., 2009 | Wheat |
| Fluorene   | 4.18 | 5.71   | 166.22 | C1C2=CC=CC=C2C3=CC=CC=C3 | 1.14          | 1.61        | -0.55        | Tao et al., 2009 | Wheat |
| Fluorene   | 4.18 | 3.47   | 166.22 | C1C2=CC=CC=C2C3=CC=CC=C3 | 1.14          | 1.59        | -0.35        | Tao et al., 2009 | Wheat |
| Fluorene   | 4.18 | 5.31   | 166.22 | C1C2=CC=CC=C2C3=CC=CC=C3 | 1.14          | 1.73        | -0.40        | Tao et al., 2009 | Wheat |
| Fluorene   | 4.18 | 3.47   | 166.22 | C1C2=CC=CC=C2C3=CC=CC=C3 | 1.14          | 1.46        | -0.48        | Tao et al., 2009 | Wheat |
| Fluorene   | 4.18 | 6.22   | 166.22 | C1C2=CC=CC=C2C3=CC=CC=C3 | 1.14          | 1.53        | -0.66        | Tao et al., 2009 | Wheat |
| Fluorene   | 4.18 | 4.81   | 166.22 | C1C2=CC=CC=C2C3=CC=CC=C3 | 1.14          | 1.88        | -0.20        | Tao et al., 2009 | Wheat |
| Fluorene   | 4.18 | 2.67   | 166.22 | C1C2=CC=CC=C2C3=CC=CC=C3 | 1.14          | 1.71        | -0.12        | Tao et al., 2009 | Wheat |
| Fluorene   | 4.18 | 4.16   | 166.22 | C1C2=CC=CC=C2C3=CC=CC=C3 | 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=C3 | 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=C3 | 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=C3 | 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=C3 | 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=C3 | 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=C3 | 1.14          | 1.96        | -0.14        | Tao et al., 2009 | Wheat |
| Compound  | Concentration 1 | Concentration 2 | MW | Formula 1 | Concentration 3 | Concentration 4 | MW | Concentration 5 | Concentration 6 |
|-----------|----------------|----------------|----|-----------|----------------|----------------|----|----------------|----------------|
| Phenanthrene | 4.46 | 3.47 | 178.23 | C1=CC=C2C(=C1)C=C3=CC=CC=C3 | 1.14 | 1.68 | -0.54 | Tao et al., 2009 | Wheat |
| Phenanthrene | 4.46 | 5.31 | 178.23 | C1=CC=C2C(=C1)C=C3=CC=CC=C3 | 1.14 | 1.85 | -0.56 | Tao et al., 2009 | Wheat |
| Phenanthrene | 4.46 | 6.22 | 178.23 | C1=CC=C2C(=C1)C=C3=CC=CC=C3 | 1.14 | 1.75 | -0.72 | Tao et al., 2009 | Wheat |
| Phenanthrene | 4.46 | 4.81 | 178.23 | C1=CC=C2C(=C1)C=C3=CC=CC=C3 | 1.14 | 2.01 | -0.36 | Tao et al., 2009 | Wheat |
| Phenanthrene | 4.46 | 2.67 | 178.23 | C1=CC=C2C(=C1)C=C3=CC=CC=C3 | 1.14 | 1.89 | -0.22 | Tao et al., 2009 | Wheat |
| Phenanthrene | 4.46 | 4.74 | 178.23 | C1=CC=C2C(=C1)C=C3=CC=CC=C3 | 1.14 | 1.89 | -0.47 | Tao et al., 2009 | Wheat |
| Phenanthrene | 4.46 | 4.16 | 178.23 | C1=CC=C2C(=C1)C=C3=CC=CC=C3 | 1.14 | 1.89 | -0.41 | Tao et al., 2009 | Wheat |
| Anthracene | 4.54 | 5.31 | 178.23 | C1=CC=C2C=C3=C=C3=CC=CC2=C1 | 1.14 | 1.62 | -0.87 | Tao et al., 2009 | Wheat |
| Anthracene | 4.54 | 1.41 | 178.23 | C1=CC=C2C=C3=C=C3=CC2=C1 | 1.14 | 1.69 | -0.22 | Tao et al., 2009 | Wheat |
| Anthracene | 4.54 | 2.71 | 178.23 | C1=CC=C2C=C3=C=C3=CC2=C1 | 1.14 | 1.95 | -0.24 | Tao et al., 2009 | Wheat |
| Anthracene | 4.54 | 5.71 | 178.23 | C1=CC=C2C=C3=C=C3=CC2=C1 | 1.14 | 1.82 | -0.70 | Tao et al., 2009 | Wheat |
| Anthracene | 4.54 | 2.60 | 178.23 | C1=CC=C2C=C3=C=C3=CC2=C1 | 1.14 | 1.67 | -0.51 | Tao et al., 2009 | Wheat |
| Anthracene | 4.54 | 3.47 | 178.23 | C1=CC=C2C=C3=C=C3=CC2=C1 | 1.14 | 1.97 | -0.34 | Tao et al., 2009 | Wheat |
| Anthracene | 4.54 | 5.31 | 178.23 | C1=CC=C2C=C3=C=C3=CC2=C1 | 1.14 | 2.10 | -0.39 | Tao et al., 2009 | Wheat |
| Anthracene | 4.54 | 3.47 | 178.23 | C1=CC=C2C=C3=C=C3=CC2=C1 | 1.14 | 1.35 | -0.95 | Tao et al., 2009 | Wheat |
| Anthracene | 4.54 | 6.22 | 178.23 | C1=CC=C2C=C3=C=C3=CC2=C1 | 1.14 | 1.89 | -0.66 | Tao et al., 2009 | Wheat |
| Anthracene | 4.54 | 4.81 | 178.23 | C1=CC=C2C=C3=C=C3=CC2=C1 | 1.14 | 2.15 | -0.29 | Tao et al., 2009 | Wheat |
| Anthracene | 4.54 | 4.74 | 178.23 | C1=CC=C2C=C3=C=C3=CC2=C1 | 1.14 | 2.09 | -0.35 | Tao et al., 2009 | Wheat |
| Compound          | n  | m/z  | molar mass | F-IR-MS   | F-IR-MS   | Retention Time | Source       | Plant  |
|-------------------|----|------|------------|-----------|-----------|---------------|-------------|--------|
| Anthracene        | 4.54 | 4.16 | 178.23     | C1=CC=C2=C3=C=CC3=CC2=C1 | 1.14 | 2.09 | -0.29 | Tao et al., 2009 | Wheat |
| Fluoranthene      | 5.16 | 1.41 | 202.25     | C1=CC=C2(C=CC1)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=C2(C=CC1)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=C2(C=CC1)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=C2(C=CC1)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=C2(C=CC1)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=CC=C2=C3=C=CC3=C=CC4=CC(=C43)C=C2 | 1.14 | 2.42 | -0.13 | Tao et al., 2009 | Wheat |
| Pyrene            | 5.18 | 4.33 | 202.25     | C1=CC=C2=C3=C=CC3=C=CC4=CC(=C43)C=C2 | 1.14 | 2.54 | -0.50 | Tao et al., 2009 | Wheat |
| Pyrene            | 5.18 | 5.71 | 202.25     | C1=CC=C2=C3=C=CC3=C=CC4=CC(=C43)C=C2 | 1.14 | 2.63 | -0.53 | Tao et al., 2009 | Wheat |
| Pyrene            | 5.18 | 3.47 | 202.25     | C1=CC=C2=C3=C=CC3=C=CC4=CC(=C43)C=C2 | 1.14 | 2.66 | -0.28 | Tao et al., 2009 | Wheat |
| Pyrene            | 5.18 | 5.31 | 202.25     | C1=CC=C2=C3=C=CC3=C=CC4=CC(=C43)C=C2 | 1.14 | 2.53 | -0.60 | Tao et al., 2009 | Wheat |
| Pyrene            | 5.18 | 6.22 | 202.25     | C1=CC=C2=C3=C=CC3=C=CC4=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=C2=C(C=CC1)C=C3=CC4=CC=C=C=C=C=C=C4=C=C32 | 1.14 | 3.09 | 0.11  | Tao et al., 2009 | Wheat |
| Benzo[a]anthracene| 5.61 | 4.33 | 228.3      | C1=CC=C2=C(C=CC1)C=C3=CC4=CC=C=C=C=C=C=C4=C=C32 | 1.14 | 3.03 | -0.44 | Tao et al., 2009 | Wheat |

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| Compound         | Value 1 | Value 2 | Value 3 | Formula                                                                 | Charge 1 | Charge 2 | Charge 3 | References       | Crop               |
|------------------|---------|---------|---------|--------------------------------------------------------------------------|----------|----------|----------|------------------|--------------------|
| Benzo[a]anthracene | 5.61    | 5.31    | 228.3   | C1=CC=C2C(=C1)C=CC3=CC4=CC=C=C=C=C4=C=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=C=C=C=C4=C=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=CC2=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=CC2=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=CC2=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=CC2=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=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=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=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=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=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=C=C)C5C3=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=C=C)C5C3=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=C=C)C5C3=CC2=C1                           | 1.14     | 3.14     | -1.04    | Tao et al., 2009 | Wheat              |
| Compound                 | Mass | LogP | Retention Time | CAS Registry | Ref | Type |
|-------------------------|------|------|----------------|--------------|-----|------|
| Benzo[k]fluoranthene    | 252.3| 3.47 | 6.20           | 6.20         | Tao et al., 2009 | Wheat |
| Benzo[k]fluoranthene    | 252.3| 5.31 | 6.20           | 6.20         | Tao et al., 2009 | Wheat |
| Benzo[k]fluoranthene    | 252.3| 3.47 | 6.20           | 6.20         | Tao et al., 2009 | Wheat |
| Benzo[k]fluoranthene    | 252.3| 6.22 | 6.20           | 6.20         | Tao et al., 2009 | Wheat |
| Benzo[k]fluoranthene    | 252.3| 4.74 | 6.20           | 6.20         | Tao et al., 2009 | Wheat |
| Benzo[a]pyrene          | 252.3| 5.31 | 6.41           | 6.41         | Tao et al., 2009 | Wheat |
| Benzo[a]pyrene          | 252.3| 4.33 | 6.41           | 6.41         | Tao et al., 2009 | Wheat |
| Benzo[a]pyrene          | 252.3| 5.71 | 6.41           | 6.41         | Tao et al., 2009 | Wheat |
| Benzo[a]pyrene          | 252.3| 3.47 | 6.41           | 6.41         | Tao et al., 2009 | Wheat |
| Benzo[a]pyrene          | 252.3| 6.22 | 6.41           | 6.41         | Tao et al., 2009 | Wheat |
| Dibenzo[a,h]anthracene  | 278.3| 4.33 | 6.75           | 6.75         | Tao et al., 2009 | Wheat |
| Dibenzo[a,h]anthracene  | 278.3| 2.71 | 6.75           | 6.75         | Tao et al., 2009 | Wheat |
| Dibenzo[a,h]anthracene  | 278.3| 2.60 | 6.75           | 6.75         | Tao et al., 2009 | Wheat |
| Dibenzo[a,h]anthracene  | 278.3| 3.47 | 6.75           | 6.75         | Tao et al., 2009 | Wheat |

Tao et al., 2009
Wheat
| Compound                     | Log P | Octanol/Water | Molecular Weight | Molecular Structure                                                                 | Delta G | Delta H | Delta S | Source       | Crop         |
|------------------------------|-------|---------------|------------------|-------------------------------------------------------------------------------------|---------|---------|---------|--------------|--------------|
| Dibenzo[a,h]anthracene       | 6.75  | 5.31          | 278.3            | C1=CC=C2C(=C1)C=CC3=CC4=C(C=C5)C5=CC=CC=C54C=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=C5)C5=CC=CC=C54C=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=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=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=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=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=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                                                        | 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                                  | 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                                                      | 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)Cl2=CC(=C(C=C2Cl)Cl)Cl)Cl                                    | 1.00    | 3.20    | 0.07    | Trapp et al., 1990 | Barely      |
| Compound          | Log P  | Henry's law coefficient | Henry's constant | Source                     | Plant   |
|-------------------|--------|-------------------------|-----------------|---------------------------|---------|
| DDT               | 6.36   | 3.55                    | 354.5           |                           |         |
| Phenanthrene      | 4.46   | 2.00                    | 178.23          |                           |         |
| Anthracene        | 4.54   | 2.00                    | 178.23          |                           |         |
| Fluoranthene      | 5.16   | 2.00                    | 202.25          |                           |         |
| Pyrene            | 5.18   | 2.00                    | 202.25          |                           |         |
| Benzo[a]anthracene| 5.61   | 2.00                    | 228.3           |                           |         |
| Chrysene          | 5.73   | 2.00                    | 228.3           |                           |         |
| Benzo[e]pyrene    | 6.44   | 2.00                    | 252.3           |                           |         |
| Benzo[b]fluoranthene| 5.78  | 2.00                    | 252.3           |                           |         |
| Benzo[k]fluoranthene| 6.20  | 2.00                    | 252.3           |                           |         |
| Benzo[a]pyrene    | 6.41   | 2.00                    | 252.3           |                           |         |
| Dibenz[a,h]anthracene| 6.75| 2.00                    | 278.3           |                           |         |
| Benz[phi]perylene | 6.90   | 2.00                    | 276.3           |                           |         |
| Compound          | Carrot | Barely | Radish | Carrot | Barely | Radish |
|------------------|--------|--------|--------|--------|--------|--------|
| Indeno[1,2,3-cd]pyrene | 6.70   | 5.90   | 5.90   | 5.70   | 5.70   | 4.90   |
| Galaxolide       | 2.00   | 1.55   | 13.80  | 1.55   | 1.55   | 3.80   |
| Galaxolide       | 258.4  | 258.4  | 289.5  | 289.5  | 289.5  | 315.6  |
| Tonalide         | 0.24   | 1.00   | 0.24   | 1.00   | 1.00   | 0.10   |
| Tonalide         | 2.43   | 1.66   | 1.26   | 1.74   | 1.74   | 0.91   |
| Triclocarban     | 6.29   | 4.80   | 4.80   | 4.80   | 4.80   | 0.91   |
| Triclosan        | 276.3  | 258.4  | 289.5  | 289.5  | 289.5  | 315.6  |
| Triclosan        | 0.24   | 1.00   | 0.24   | 1.00   | 1.00   | 0.24   |
| Triclosan        | 2.43   | 1.69   | 1.26   | 1.74   | 1.74   | 0.91   |
| Triclosan        | 0.24   | 1.00   | 0.24   | 1.00   | 1.00   | 0.24   |
| Triclosan        | 0.24   | 1.00   | 0.24   | 1.00   | 1.00   | 0.24   |
| Trimethoprim     | 0.91   | 0.91   | 0.91   | 0.91   | 0.91   | 0.91   |
| Carbamazepine    | 2.45   | 1.72   | 236.27 | 1.72   | 1.72   | 236.27 |
| BDE-66           | 0.24   | 0.24   | 0.24   | 0.24   | 0.24   | 0.24   |
| BDE-66           | 0.24   | 0.24   | 0.24   | 0.24   | 0.24   | 0.24   |
| BDE-66           | 0.24   | 0.24   | 0.24   | 0.24   | 0.24   | 0.24   |
| BDE-66           | 0.24   | 0.24   | 0.24   | 0.24   | 0.24   | 0.24   |

Kipoupolou et al., 1999
Macherius et al., 2012
Macherius et al., 2012
Macherius et al., 2012
Macherius et al., 2012
Macherius et al., 2012
Wu et al., 2012
Pannu et al., 2012
Proser et al., 2014
Proser et al., 2014
Boxall et al., 2006
Carter et al., 2014
Huang et al., 2011
Huang et al., 2011
Huang et al., 2011

| BDE-66 | 6.29 | 3.19 | 485.79 | C1=CC(=C(C\text{=C1}O\text{C}2=C(C=C(C=C2)Br \hspace{1cm} \text{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\text{=C1}O\text{C}2=C(C=C(C=C2)Br \hspace{1cm} \text{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\text{=C1}O\text{C}2=C(C=C(C=C2)Br \hspace{1cm} \text{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\text{=C1}O\text{C}2=C(C=C(C=C2)Br \hspace{1cm} \text{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\text{=C1}O\text{C}2=C(C=C(C=C2)Br \hspace{1cm} \text{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\text{=C1}O\text{C}2=C(C=C(C=C2)Br \hspace{1cm} \text{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\text{=C1}Br)Br)OC2=C(C(\text{=C(C=C}2)Br)Br)Br | 0.70 | -1.43 | Huang et al., 2011 | Pumpkin |
| BDE-85 | 6.69 | 1.90 | 564.7 | C1=CC(=C(C\text{=C1}Br)Br)OC2=C(C(\text{=C(C=C}2)Br)Br)Br | 0.53 | -1.40 | Huang et al., 2011 | Maize |
| BDE-85 | 6.69 | 1.90 | 564.7 | C1=CC(=C(C\text{=C1}Br)Br)OC2=C(C(\text{=C(C=C}2)Br)Br)Br | 0.56 | -1.33 | Huang et al., 2011 | Ryegrass |
| BDE-85 | 6.69 | 3.19 | 564.7 | C1=CC(=C(C\text{=C1}Br)Br)OC2=C(C(\text{=C(C=C}2)Br)Br)Br | 0.70 | -1.17 | Huang et al., 2011 | Pumpkin |
| BDE-85 | 6.69 | 3.19 | 564.7 | C1=CC(=C(C\text{=C1}Br)Br)OC2=C(C(\text{=C(C=C}2)Br)Br)Br | 0.53 | -1.01 | Huang et al., 2011 | Maize |
| BDE-85 | 6.69 | 3.19 | 564.7 | C1=CC(=C(C\text{=C1}Br)Br)OC2=C(C(\text{=C(C=C}2)Br)Br)Br | 0.56 | -1.24 | Huang et al., 2011 | Ryegrass |
| BDE-85 | 6.69 | 0.98 | 564.7 | C1=CC(=C(C\text{=C1}Br)Br)OC2=C(C(\text{=C(C=C}2)Br)Br)Br | 0.70 | -1.14 | Huang et al., 2011 | Pumpkin |
| BDE-85 | 6.69 | 0.98 | 564.7 | C1=CC(=C(C\text{=C1}Br)Br)OC2=C(C(\text{=C(C=C}2)Br)Br)Br | 0.53 | -1.10 | Huang et al., 2011 | Maize |
| Compound | Mass (amu) | Intensity (arb. units) | Retention Time (min) | Spectrum | References | Plant Species |
|----------|-----------|------------------------|----------------------|----------|------------|---------------|
| BDE-85  | 6.69      | 0.98                   | 564.7                | C1=C(C=C(C1Br)Br)OC2=C(C(=C(C=C2Br)Br)Br)Br | 0.56     | -1.06        | Huang et al., 2011 | Ryegrass |
| BDE-191 | 7.49      | 3.19                   | 722.5                | C1=C(C=C(C1Br)Br)BrOC2=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(C1Br)Br)BrOC2=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(C1Br)Br)BrOC2=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(C1Br)Br)BrOC2=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(C1Br)Br)BrOC2=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(C1Br)Br)BrOC2=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(C1Br)Br)BrOC2=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(C1Br)Br)BrOC2=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(C1Br)Br)BrOC2=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(C1Br)Br)BrOC2=C(C(=C(C=C2Br)Br)Br)Br | 0.70     | -1.43        | Huang et al., 2011 | Pumpkin |
| BDE-197 | 7.90      | 3.19                   | 801.4                | C1=C(C=C(C1Br)Br)BrOC2=C(C(=C(C=C2Br)Br)Br)Br | 0.53     | -1.38        | Huang et al., 2011 | Maize |
| BDE-197 | 7.90      | 3.19                   | 801.4                | C1=C(C=C(C1Br)Br)BrOC2=C(C(=C(C=C2Br)Br)Br)Br | 0.56     | -1.19        | Huang et al., 2011 | Ryegrass |
| BDE-197 | 7.90      | 1.90                   | 801.4                | C1=C(C=C(C1Br)Br)BrOC2=C(C(=C(C=C2Br)Br)Br)Br | 0.70     | -1.08        | Huang et al., 2011 | Pumpkin |

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| Compound | 
| --- | --- | --- | --- | --- |
| **BDE-197** | 7.90 | 1.90 | 801.4 | \( C_1=\text{C}(=\text{C}(\text{=C}(\text{=C}1\text{Br})\text{Br})\text{Br})\text{OC}2=\text{C}(\text{=}\text{C}(\text{=}\text{C}2\text{Br})\text{Br})\text{Br})\text{Br} \) | 0.53 | -1.18 | Huang et al., 2011 | Maize |
| **BDE-197** | 7.90 | 1.90 | 801.4 | \( C_1=\text{C}(=\text{C}(\text{=}\text{C}1\text{Br})\text{Br})\text{Br})\text{OC}2=\text{C}(\text{=}\text{C}(\text{=}\text{C}2\text{Br})\text{Br})\text{Br})\text{Br} \) | 0.56 | -1.49 | Huang et al., 2011 | Ryegrass |
| **BDE-197** | 7.90 | 0.98 | 801.4 | \( C_1=\text{C}(=\text{C}(\text{=}\text{C}1\text{Br})\text{Br})\text{Br})\text{OC}2=\text{C}(\text{=}\text{C}(\text{=}\text{C}2\text{Br})\text{Br})\text{Br})\text{Br} \) | 0.70 | -1.32 | Huang et al., 2011 | Pumpkin |
| **BDE-197** | 7.90 | 0.98 | 801.4 | \( C_1=\text{C}(=\text{C}(\text{=}\text{C}1\text{Br})\text{Br})\text{Br})\text{OC}2=\text{C}(\text{=}\text{C}(\text{=}\text{C}2\text{Br})\text{Br})\text{Br})\text{Br} \) | 0.53 | -1.42 | Huang et al., 2011 | Maize |
| **BDE-197** | 7.90 | 0.98 | 801.4 | \( C_1=\text{C}(=\text{C}(\text{=}\text{C}1\text{Br})\text{Br})\text{Br})\text{OC}2=\text{C}(\text{=}\text{C}(\text{=}\text{C}2\text{Br})\text{Br})\text{Br})\text{Br} \) | 0.56 | -1.68 | Huang et al., 2011 | Ryegrass |
| **BDE-208** | 8.30 | 3.19 | 880.3 | \( C_1=\text{C}(=\text{C}(\text{=}\text{C}1\text{Br})\text{Br})\text{Br})\text{OC}2=\text{C}(\text{=}\text{C}(\text{=}\text{C}2\text{Br})\text{Br})\text{Br})\text{Br} \) | 0.70 | -2.02 | Huang et al., 2011 | Pumpkin |
| **BDE-208** | 8.30 | 1.90 | 880.3 | \( C_1=\text{C}(=\text{C}(\text{=}\text{C}1\text{Br})\text{Br})\text{Br})\text{OC}2=\text{C}(\text{=}\text{C}(\text{=}\text{C}2\text{Br})\text{Br})\text{Br})\text{Br} \) | 0.70 | -2.16 | Huang et al., 2011 | Pumpkin |
| **BDE-208** | 8.30 | 1.90 | 880.3 | \( C_1=\text{C}(=\text{C}(\text{=}\text{C}1\text{Br})\text{Br})\text{Br})\text{OC}2=\text{C}(\text{=}\text{C}(\text{=}\text{C}2\text{Br})\text{Br})\text{Br})\text{Br} \) | 0.53 | -2.13 | Huang et al., 2011 | Maize |
| **BDE-208** | 8.30 | 1.90 | 880.3 | \( C_1=\text{C}(=\text{C}(\text{=}\text{C}1\text{Br})\text{Br})\text{Br})\text{OC}2=\text{C}(\text{=}\text{C}(\text{=}\text{C}2\text{Br})\text{Br})\text{Br})\text{Br} \) | 0.56 | -2.34 | Huang et al., 2011 | Ryegrass |
| **BDE-208** | 8.30 | 0.98 | 880.3 | \( C_1=\text{C}(=\text{C}(\text{=}\text{C}1\text{Br})\text{Br})\text{Br})\text{OC}2=\text{C}(\text{=}\text{C}(\text{=}\text{C}2\text{Br})\text{Br})\text{Br})\text{Br} \) | 0.70 | -2.30 | Huang et al., 2011 | Pumpkin |
| **BDE-208** | 8.30 | 0.98 | 880.3 | \( C_1=\text{C}(=\text{C}(\text{=}\text{C}1\text{Br})\text{Br})\text{Br})\text{OC}2=\text{C}(\text{=}\text{C}(\text{=}\text{C}2\text{Br})\text{Br})\text{Br})\text{Br} \) | 0.53 | -2.30 | Huang et al., 2011 | Maize |
| **BDE-208** | 8.30 | 0.98 | 880.3 | \( C_1=\text{C}(=\text{C}(\text{=}\text{C}1\text{Br})\text{Br})\text{Br})\text{OC}2=\text{C}(\text{=}\text{C}(\text{=}\text{C}2\text{Br})\text{Br})\text{Br})\text{Br} \) | 0.56 | -2.40 | Huang et al., 2011 | Ryegrass |
| **BDE-207** | 8.30 | 3.19 | 880.3 | \( C_1=\text{C}(=\text{C}(\text{=}\text{C}1\text{Br})\text{Br})\text{Br})\text{OC}2=\text{C}(\text{=}\text{C}(\text{=}\text{C}2\text{Br})\text{Br})\text{Br})\text{Br} \) | 0.70 | -1.26 | Huang et al., 2011 | Pumpkin |
| **BDE-207** | 8.30 | 3.19 | 880.3 | \( C_1=\text{C}(=\text{C}(\text{=}\text{C}1\text{Br})\text{Br})\text{Br})\text{OC}2=\text{C}(\text{=}\text{C}(\text{=}\text{C}2\text{Br})\text{Br})\text{Br})\text{Br} \) | 0.53 | -1.49 | Huang et al., 2011 | Maize |

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| Chemical          | Mass  | RT   | P/V  | Concentration | Reference       | Plant     |
|-------------------|-------|------|------|---------------|-----------------|-----------|
| BDE-207           | 8.30  | 3.19 | 880.3| 0.56          | -1.60           | Huang et al., 2011 | Ryegrass |
|                   |       |      |      |               |                 |           |
|                   | 8.30  | 1.90 | 880.3| 0.70          | -2.60           | Huang et al., 2011 | Pumpkin |
|                   |       |      |      |               |                 |           |
|                   | 8.30  | 1.90 | 880.3| 0.53          | -2.15           | Huang et al., 2011 | Maize   |
|                   |       |      |      |               |                 |           |
|                   | 8.30  | 0.98 | 880.3| 0.70          | -2.01           | Huang et al., 2011 | Pumpkin |
|                   |       |      |      |               |                 |           |
|                   | 8.30  | 0.98 | 880.3| 0.53          | -1.74           | Huang et al., 2011 | Maize   |
|                   |       |      |      |               |                 |           |
| alpha-endosulfan  | 0.50  | 8.80 | 406.9| 0.56          | -1.92           | Huang et al., 2011 | Ryegrass |
| endosulfan sulfate| 0.56  | 8.80 | 422.9| 0.10          | -0.61           | GONZALEZ et al., 2003 | leek |
| dieldrin          | 0.72  | 8.80 | 380.9| 0.10          | -0.66           | GONZALEZ et al., 2003 | leek |
| heptachlor        | 0.72  | 8.80 | 373.3| 0.10          | 0.22            | GONZALEZ et al., 2003 | leek |
| heptachlor epoxide| 0.62  | 8.80 | 389.3| 0.10          | -0.87           | GONZALEZ et al., 2003 | leek |
| Imidacloprid      | 0.57  | 3.05 | 255.66| 0.53         | -0.31           | Wang et al., 2020 | Maize   |
| Acetamiprid       | 0.80  | 3.05 | 222.67| 0.53         | -0.18           | Wang et al., 2020 | Maize   |
| Tricyclazole      | 1.70  | 3.05 | 189.24| 0.53         | -0.24           | Wang et al., 2020 | Maize   |

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

| Parameter          | Values                               |
|--------------------|--------------------------------------|
| 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