**Supplementary Material**

**Predicting crop root concentration factors of organic contaminants with machine learning models**

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#Equal contribution

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Supplemental Methods:

**Five-fold cross validation**

The whole dataset was shuffled and randomly split into 5 equal groups. Each group was used as a test set whereby the model was trained using the other four groups of data. To fine-tune the model and select the best parameter sets, 12.5% of the training data (10% of the whole dataset) were used as a validation set while the other 87.5% of the training data (80% of whole dataset) were used to train the model. The best parameter sets were retrieved by examining the performance of trained models on the validation set. The best combination of parameters was then used to build the model and test on the unseen test set. The final prediction results were then averaged based on the 5 model performance. Therefore, each sample is given the opportunity to be tested once and used to train the model four times.

**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



Figure S1: Predicting root concentration factor (RCF) using linear regression model.

**Table S1. Dataset of chemical, soil, and plant properties, and root concentration factors (RCF).** fom: Soil organic matter content; MW: Molecular weight; flipid: Root lipid content; E: Excess molar refractivity; S: Dipolarity/polarizability; A: Hydrogen bond acidity; B: Hydrogen bond basicity; V: Molecular volume.

|  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Compounds** | **MW** | **E** | **S** | **A** | **B** | **V** | **fom (%)** | **flipid (%)** | **log RCF-soil** | **Citation** | **Plant** |
| Penconazole | 284.18 | 1.55 | 1.75 | 0 | 0.93 | 2.0523 | 0.97 | 1.1 | -0.03 | Jiang et al., 2016 | Wheat |
| Penconazole | 284.18 | 1.55 | 1.75 | 0 | 0.93 | 2.0523 | 3.26 | 1.1 | -0.19 | Jiang et al., 2016 | Wheat |
| Penconazole | 284.18 | 1.55 | 1.75 | 0 | 0.93 | 2.0523 | 5.03 | 1.1 | -0.3 | Jiang et al., 2016 | Wheat |
| Penconazole | 284.18 | 1.55 | 1.75 | 0 | 0.93 | 2.0523 | 1.59 | 1.1 | -0.13 | Jiang et al., 2016 | Wheat |
| Penconazole | 284.18 | 1.55 | 1.75 | 0 | 0.93 | 2.0523 | 2.6 | 1.1 | -0.25 | Jiang et al., 2016 | Wheat |
| Aldrin  | 364.9 | 2.07 | 0.95 | 0 | 0.42 | 2.0134 | 3.6 | 0.24 | -1.38 | Harris and Sans, 1967 | Carrot |
| Aldrin  | 364.9 | 2.07 | 0.95 | 0 | 0.42 | 2.0134 | 66.5 | 0.24 | -2.92 | Harris and Sans, 1967 | Carrot |
| Dieldrin | 380.9 | 2.09 | 1.57 | 0 | 0.75 | 2.0065 | 1.4 | 0.24 | -0.6 | Harris and Sans, 1967 | Carrot |
| Dieldrin | 380.9 | 2.09 | 1.57 | 0 | 0.75 | 2.0065 | 3.6 | 0.24 | -0.99 | Harris and Sans, 1967 | Carrot |
| Dieldrin | 380.9 | 2.09 | 1.57 | 0 | 0.75 | 2.0065 | 66.5 | 0.24 | -2.29 | Harris and Sans, 1967 | Carrot |
| Dieldrin | 380.9 | 2.09 | 1.57 | 0 | 0.75 | 2.0065 | 3.6 | 0.1 | -1.33 | Harris and Sans, 1967 | Radish |
| Dieldrin | 380.9 | 2.09 | 1.57 | 0 | 0.75 | 2.0065 | 66.5 | 0.1 | -2.59 | Harris and Sans, 1967 | Radish |
| Dieldrin | 380.9 | 2.09 | 1.57 | 0 | 0.75 | 2.0065 | 3.6 | 0.1 | -1.56 | Harris and Sans, 1967 | Turnips |
| m-DCB (1,3-DCB) | 147 | 0.85 | 0.73 | 0 | 0.02 | 0.9612 | 2.82 | 0.34 | 0.22 | Zhang et al., 2005 | Spinach |
| m-DCB (1,3-DCB) | 147 | 0.85 | 0.73 | 0 | 0.02 | 0.9612 | 0.78 | 0.34 | 0.61 | Zhang et al., 2005 | Spinach |
| m-DCB (1,3-DCB) | 147 | 0.85 | 0.73 | 0 | 0.02 | 0.9612 | 1.41 | 0.24 | -0.03 | Zhang et al., 2005 | Carrot |
| m-DCB (1,3-DCB) | 147 | 0.85 | 0.73 | 0 | 0.02 | 0.9612 | 0.78 | 0.24 | -0.12 | Zhang et al., 2005 | Carrot |
| m-DCB (1,3-DCB) | 147 | 0.85 | 0.73 | 0 | 0.02 | 0.9612 | 2.82 | 0.09 | -0.59 | Zhang et al., 2005 | Radish |
| m-DCB (1,3-DCB) | 147 | 0.85 | 0.73 | 0 | 0.02 | 0.9612 | 0.78 | 0.09 | -0.15 | Zhang et al., 2005 | Radish |
| p-DCB (1,4-DCB) | 147 | 0.83 | 0.75 | 0 | 0.02 | 0.9612 | 2.82 | 0.34 | 0.14 | Zhang et al., 2005 | Spinach |
| p-DCB (1,4-DCB) | 147 | 0.83 | 0.75 | 0 | 0.02 | 0.9612 | 1.41 | 0.34 | -0.12 | Zhang et al., 2005 | Spinach |
| p-DCB (1,4-DCB) | 147 | 0.83 | 0.75 | 0 | 0.02 | 0.9612 | 1.41 | 0.09 | -0.38 | Zhang et al., 2005 | Radish |
| o-DCB (1,2-DCB) | 147 | 0.87 | 0.78 | 0 | 0.04 | 0.9612 | 0.78 | 0.34 | 0.7 | Zhang et al., 2005 | Spinach |
| o-DCB (1,2-DCB) | 147 | 0.87 | 0.78 | 0 | 0.04 | 0.9612 | 0.78 | 0.24 | 0 | Zhang et al., 2005 | Carrot |
| o-DCB (1,2-DCB) | 147 | 0.87 | 0.78 | 0 | 0.04 | 0.9612 | 0.78 | 0.09 | -0.18 | Zhang et al., 2005 | Radish |
| 1,2,4-TCB | 181.4 | 0.98 | 0.81 | 0 | 0 | 1.0836 | 2.82 | 0.34 | -0.41 | Zhang et al., 2005 | Spinach |
| 1,2,4-TCB | 181.4 | 0.98 | 0.81 | 0 | 0 | 1.0836 | 1.41 | 0.34 | -0.1 | Zhang et al., 2005 | Spinach |
| 1,2,4-TCB | 181.4 | 0.98 | 0.81 | 0 | 0 | 1.0836 | 2.82 | 0.17 | -0.35 | Zhang et al., 2005 | Celery |
| 1,2,4-TCB | 181.4 | 0.98 | 0.81 | 0 | 0 | 1.0836 | 1.41 | 0.17 | -0.2 | Zhang et al., 2005 | Celery |
| 1,2,4-TCB | 181.4 | 0.98 | 0.81 | 0 | 0 | 1.0836 | 0.78 | 0.17 | -0.08 | Zhang et al., 2005 | Celery |
| 1,2,4-TCB | 181.4 | 0.98 | 0.81 | 0 | 0 | 1.0836 | 1.41 | 0.24 | -0.41 | Zhang et al., 2005 | Carrot |
| 1,2,4-TCB | 181.4 | 0.98 | 0.81 | 0 | 0 | 1.0836 | 2.82 | 0.09 | -0.94 | Zhang et al., 2005 | Radish |
| 1,2,4-TCB | 181.4 | 0.98 | 0.81 | 0 | 0 | 1.0836 | 1.41 | 0.09 | -0.76 | Zhang et al., 2005 | Radish |
| Fluorene | 166.22 | 1.59 | 1.061 | 0 | 0.24 | 1.357 | 12.72 | 0.1 | -1.59 | Cai et al., 2008 | Radish |
| Phenanthrene | 178.23 | 2.06 | 1.29 | 0 | 0.26 | 1.4544 | 12.72 | 0.1 | -1.45 | Cai et al., 2008 | Radish |
| Phenanthrene | 178.23 | 2.06 | 1.29 | 0 | 0.26 | 1.4544 | 4.84 | 0.1 | -1.05 | Cai et al., 2008 | Radish |
| Anthracene | 178.23 | 2.29 | 1.34 | 0 | 0.28 | 1.4544 | 3.78 | 0.1 | -1.63 | Cai et al., 2008 | Radish |
| Anthracene | 178.23 | 2.29 | 1.34 | 0 | 0.28 | 1.4544 | 12.72 | 0.1 | -2.15 | Cai et al., 2008 | Radish |
| Fluoranthene | 202.25 | 2.377 | 1.55 | 0 | 0.24 | 1.585 | 0.79 | 0.1 | -0.72 | Cai et al., 2008 | Radish |
| Benzo[a]pyrene | 252.3 | 3.63 | 1.98 | 0 | 0.44 | 1.9536 | 3.78 | 0.1 | -2.52 | Cai et al., 2008 | Radish |
| Di(2-ethylhexyl) phthalate | 390.6 | 0.64 | 1.25 | 0 | 1.02 | 3.4014 | 6.76 | 0.1 | -1.94 | Cai et al., 2008 | Radish |
| Di(2-ethylhexyl) phthalate | 390.6 | 0.64 | 1.25 | 0 | 1.02 | 3.4014 | 12.72 | 0.1 | -2.4 | Cai et al., 2008 | Radish |
| Phenanthrene | 178.23 | 2.06 | 1.29 | 0 | 0.26 | 1.4544 | 1.45 | 0.68 | -0.88 | Gao et al., 2005 | Chinese cabbage |
| Phenanthrene | 178.23 | 2.06 | 1.29 | 0 | 0.26 | 1.4544 | 1.45 | 0.32 | -1.15 | Gao et al., 2005 | Amaranth |
| Pyrene | 202.25 | 2.81 | 1.71 | 0 | 0.28 | 1.5846 | 1.45 | 0.68 | -0.26 | Gao et al., 2005 | Chinese cabbage |
| HCB | 284.8 | 1.49 | 0.99 | 0 | 0 | 1.4508 | 6.36 | 0.1 | -2.11 | Mikes et al., 2009 | Radish |
| o,p'-DDE | 318 | 1.9 | 1.5 | 0 | 0.18 | 2.0526 | 6.36 | 0.1 | -1.49 | Mikes et al., 2009 | Radish |
| p,p'-DDE | 318 | 1.8 | 1.4 | 0.06 | 0.14 | 2.0526 | 6.36 | 0.1 | -1.24 | Mikes et al., 2009 | Radish |
| o,p'-DDD | 320 | 1.8 | 1.73 | 0.1 | 0.26 | 2.0956 | 6.36 | 0.1 | -1.25 | Mikes et al., 2009 | Radish |
| p,p'-DDD | 320 | 1.76 | 1.71 | 0.02 | 0.22 | 2.0956 | 6.36 | 0.1 | -1.05 | Mikes et al., 2009 | Radish |
| o,p'-DDT | 354.5 | 1.85 | 1.7 | 0 | 0.25 | 2.218 | 6.36 | 0.1 | -1.3 | Mikes et al., 2009 | Radish |
| p,p'-DDT | 354.5 | 1.81 | 1.76 | 0 | 0.16 | 2.218 | 6.36 | 0.1 | -1.74 | Mikes et al., 2009 | Radish |
| PCB 101 | 326.4 | 2.04 | 1.61 | 0 | 0.13 | 1.9362 | 6.36 | 0.1 | -1.72 | Mikes et al., 2009 | Radish |
| PCB 153 | 360.9 | 2.18 | 1.74 | 0 | 0.11 | 2.0586 | 6.36 | 0.1 | -2.03 | Mikes et al., 2009 | Radish |
| PCB 138 | 360.9 | 2.18 | 1.74 | 0 | 0.11 | 2.0586 | 6.36 | 0.1 | -2.09 | Mikes et al., 2009 | Radish |
| PCB 180 | 395.3 | 2.29 | 1.87 | 0 | 0.09 | 2.181 | 6.36 | 0.1 | -2.07 | Mikes et al., 2009 | Radish |
| BDE-100 | 564.7 | 2.71 | 1.48 | 0 | 0.41 | 2.2579 | 3.19 | 0.53 | -1.66 | Huang et al., 2011 | Maize |
| BDE-100 | 564.7 | 2.71 | 1.48 | 0 | 0.41 | 2.2579 | 3.19 | 0.56 | -1.51 | Huang et al., 2011 | Ryegrass |
| BDE-100 | 564.7 | 2.71 | 1.48 | 0 | 0.41 | 2.2579 | 1.9 | 0.7 | -1.17 | Huang et al., 2011 | Pumpkin |
| BDE-100 | 564.7 | 2.71 | 1.48 | 0 | 0.41 | 2.2579 | 1.9 | 0.53 | -1.21 | Huang et al., 2011 | Maize |
| BDE-100 | 564.7 | 2.71 | 1.48 | 0 | 0.41 | 2.2579 | 0.98 | 0.7 | -1.07 | Huang et al., 2011 | Pumpkin |
| BDE-100 | 564.7 | 2.71 | 1.48 | 0 | 0.41 | 2.2579 | 0.98 | 0.53 | -1.05 | Huang et al., 2011 | Maize |
| BDE-153 | 643.6 | 3.09 | 1.54 | 0 | 0.52 | 2.4329 | 3.19 | 0.7 | -1.92 | Huang et al., 2011 | Pumpkin |
| BDE-153 | 643.6 | 3.09 | 1.54 | 0 | 0.52 | 2.4329 | 1.9 | 0.7 | -1.45 | Huang et al., 2011 | Pumpkin |
| BDE-153 | 643.6 | 3.09 | 1.54 | 0 | 0.52 | 2.4329 | 1.9 | 0.53 | -1.25 | Huang et al., 2011 | Maize |
| BDE-153 | 643.6 | 3.09 | 1.54 | 0 | 0.52 | 2.4329 | 0.98 | 0.7 | -1.05 | Huang et al., 2011 | Pumpkin |
| BDE-153 | 643.6 | 3.09 | 1.54 | 0 | 0.52 | 2.4329 | 0.98 | 0.53 | -1.01 | Huang et al., 2011 | Maize |
| BDE-154 | 643.6 | 3.09 | 1.5 | 0 | 0.53 | 2.4329 | 3.19 | 0.7 | -1.27 | Huang et al., 2011 | Pumpkin |
| BDE-154 | 643.6 | 3.09 | 1.5 | 0 | 0.53 | 2.4329 | 3.19 | 0.53 | -1.2 | Huang et al., 2011 | Maize |
| BDE-154 | 643.6 | 3.09 | 1.5 | 0 | 0.53 | 2.4329 | 1.9 | 0.7 | -1.23 | Huang et al., 2011 | Pumpkin |
| BDE-154 | 643.6 | 3.09 | 1.5 | 0 | 0.53 | 2.4329 | 1.9 | 0.53 | -1.33 | Huang et al., 2011 | Maize |
| BDE-154 | 643.6 | 3.09 | 1.5 | 0 | 0.53 | 2.4329 | 0.98 | 0.7 | -1.15 | Huang et al., 2011 | Pumpkin |
| BDE-154 | 643.6 | 3.09 | 1.5 | 0 | 0.53 | 2.4329 | 0.98 | 0.53 | -1.06 | Huang et al., 2011 | Maize |
| BDE-183 | 722.5 | 3.51 | 1.65 | 0 | 0.57 | 2.6079 | 3.19 | 0.7 | -1.55 | Huang et al., 2011 | Pumpkin |
| BDE-183 | 722.5 | 3.51 | 1.65 | 0 | 0.57 | 2.6079 | 3.19 | 0.53 | -1.59 | Huang et al., 2011 | Maize |
| BDE-183 | 722.5 | 3.51 | 1.65 | 0 | 0.57 | 2.6079 | 1.9 | 0.7 | -1.17 | Huang et al., 2011 | Pumpkin |
| BDE-183 | 722.5 | 3.51 | 1.65 | 0 | 0.57 | 2.6079 | 1.9 | 0.53 | -0.96 | Huang et al., 2011 | Maize |
| BDE-183 | 722.5 | 3.51 | 1.65 | 0 | 0.57 | 2.6079 | 0.98 | 0.7 | -1.7 | Huang et al., 2011 | Pumpkin |
| BDE-183 | 722.5 | 3.51 | 1.65 | 0 | 0.57 | 2.6079 | 0.98 | 0.53 | -1.52 | Huang et al., 2011 | Maize |
| BDE-28 | 406.89 | 2.07 | 1.38 | 0 | 0.27 | 1.9079 | 3.19 | 0.53 | -1.13 | Huang et al., 2011 | Maize |
| BDE-28 | 406.89 | 2.07 | 1.38 | 0 | 0.27 | 1.9079 | 1.9 | 0.53 | -0.92 | Huang et al., 2011 | Maize |
| BDE-47 | 485.79 | 2.32 | 1.45 | 0 | 0.34 | 2.0829 | 3.19 | 0.7 | -0.8 | Huang et al., 2011 | Pumpkin |
| BDE-47 | 485.79 | 2.32 | 1.45 | 0 | 0.34 | 2.0829 | 3.19 | 0.53 | -0.88 | Huang et al., 2011 | Maize |
| BDE-47 | 485.79 | 2.32 | 1.45 | 0 | 0.34 | 2.0829 | 1.9 | 0.7 | -0.64 | Huang et al., 2011 | Pumpkin |
| BDE-47 | 485.79 | 2.32 | 1.45 | 0 | 0.34 | 2.0829 | 1.9 | 0.53 | -0.75 | Huang et al., 2011 | Maize |
| BDE-47 | 485.79 | 2.32 | 1.45 | 0 | 0.34 | 2.0829 | 0.98 | 0.7 | -0.92 | Huang et al., 2011 | Pumpkin |
| BDE-47 | 485.79 | 2.32 | 1.45 | 0 | 0.34 | 2.0829 | 0.98 | 0.53 | -1.05 | Huang et al., 2011 | Maize |
| BDE-99 | 564.7 | 2.71 | 1.51 | 0 | 0.44 | 2.2579 | 3.19 | 0.7 | -1.07 | Huang et al., 2011 | Pumpkin |
| BDE-99 | 564.7 | 2.71 | 1.51 | 0 | 0.44 | 2.2579 | 3.19 | 0.53 | -1.08 | Huang et al., 2011 | Maize |
| BDE-99 | 564.7 | 2.71 | 1.51 | 0 | 0.44 | 2.2579 | 1.9 | 0.7 | -0.9 | Huang et al., 2011 | Pumpkin |
| BDE-99 | 564.7 | 2.71 | 1.51 | 0 | 0.44 | 2.2579 | 1.9 | 0.53 | -1.06 | Huang et al., 2011 | Maize |
| BDE-99 | 564.7 | 2.71 | 1.51 | 0 | 0.44 | 2.2579 | 0.98 | 0.7 | -0.98 | Huang et al., 2011 | Pumpkin |
| BDE-99 | 564.7 | 2.71 | 1.51 | 0 | 0.44 | 2.2579 | 0.98 | 0.53 | -1.05 | Huang et al., 2011 | Maize |
| Dieldrin | 380.9 | 2.09 | 1.57 | 0 | 0.75 | 2.0065 | 13.28 | 0.53 | -0.82 | Beestman et al., 1969 | Maize |
| Dieldrin | 380.9 | 2.09 | 1.57 | 0 | 0.75 | 2.0065 | 0.69 | 0.53 | 0.52 | Beestman et al., 1969 | Maize |
| Dieldrin | 380.9 | 2.09 | 1.57 | 0 | 0.75 | 2.0065 | 0.86 | 0.53 | 0.38 | Beestman et al., 1969 | Maize |
| Dieldrin | 380.9 | 2.09 | 1.57 | 0 | 0.75 | 2.0065 | 6.55 | 0.53 | -0.54 | Beestman et al., 1969 | Maize |
| Dieldrin | 380.9 | 2.09 | 1.57 | 0 | 0.75 | 2.0065 | 1.21 | 0.53 | 0.22 | Beestman et al., 1969 | Maize |
| Dieldrin | 380.9 | 2.09 | 1.57 | 0 | 0.75 | 2.0065 | 8.97 | 0.53 | -0.64 | Beestman et al., 1969 | Maize |
| 1,4-DCB | 147 | 0.83 | 0.75 | 0 | 0.02 | 0.9612 | 3.55 | 1 | 1.03 | Scheunert et al., 1994 | Barely |
| 1,2,4-TCB | 181.4 | 0.98 | 0.81 | 0 | 0 | 1.0836 | 3.55 | 1 | 0.65 | Scheunert et al., 1994 | Barely |
| 1,2,3,5-TeCB | 215.9 | 1.16 | 0.85 | 0 | 0 | 1.206 | 3.55 | 1 | 0.75 | Scheunert et al., 1994 | Barely |
| Pentachlorobeneze | 250.3 | 1.33 | 0.92 | 0.06 | 0 | 1.3284 | 3.55 | 1 | 0.03 | Scheunert et al., 1994 | Barely |
| Hexachlorobenze | 284.8 | 1.49 | 0.99 | 0 | 0 | 1.4508 | 3.55 | 1 | -0.09 | Scheunert et al., 1994 | Barely |
| Naphthalene | 128.17 | 1.34 | 0.92 | 0 | 0.2 | 1.0854 | 5.31 | 1.14 | -0.42 | Tao et al., 2009 | Wheat |
| Naphthalene | 128.17 | 1.34 | 0.92 | 0 | 0.2 | 1.0854 | 1.41 | 1.14 | -0.01 | Tao et al., 2009 | Wheat |
| Naphthalene | 128.17 | 1.34 | 0.92 | 0 | 0.2 | 1.0854 | 4.33 | 1.14 | -0.16 | Tao et al., 2009 | Wheat |
| Naphthalene | 128.17 | 1.34 | 0.92 | 0 | 0.2 | 1.0854 | 2.71 | 1.14 | 0.17 | Tao et al., 2009 | Wheat |
| Naphthalene | 128.17 | 1.34 | 0.92 | 0 | 0.2 | 1.0854 | 5.71 | 1.14 | -0.61 | Tao et al., 2009 | Wheat |
| Naphthalene | 128.17 | 1.34 | 0.92 | 0 | 0.2 | 1.0854 | 2.6 | 1.14 | -0.02 | Tao et al., 2009 | Wheat |
| Naphthalene | 128.17 | 1.34 | 0.92 | 0 | 0.2 | 1.0854 | 4.81 | 1.14 | -0.44 | Tao et al., 2009 | Wheat |
| Naphthalene | 128.17 | 1.34 | 0.92 | 0 | 0.2 | 1.0854 | 2.67 | 1.14 | -0.17 | Tao et al., 2009 | Wheat |
| Naphthalene | 128.17 | 1.34 | 0.92 | 0 | 0.2 | 1.0854 | 4.74 | 1.14 | -0.18 | Tao et al., 2009 | Wheat |
| Naphthalene | 128.17 | 1.34 | 0.92 | 0 | 0.2 | 1.0854 | 4.16 | 1.14 | -0.1 | Tao et al., 2009 | Wheat |
| Acenaphthene | 154.21 | 1.6 | 1.05 | 0 | 0.22 | 1.2586 | 4.33 | 1.14 | -0.11 | Tao et al., 2009 | Wheat |
| Acenaphthene | 154.21 | 1.6 | 1.05 | 0 | 0.22 | 1.2586 | 2.71 | 1.14 | -0.02 | Tao et al., 2009 | Wheat |
| Acenaphthene | 154.21 | 1.6 | 1.05 | 0 | 0.22 | 1.2586 | 5.71 | 1.14 | -0.68 | Tao et al., 2009 | Wheat |
| Acenaphthene | 154.21 | 1.6 | 1.05 | 0 | 0.22 | 1.2586 | 2.6 | 1.14 | -0.09 | Tao et al., 2009 | Wheat |
| Acenaphthene | 154.21 | 1.6 | 1.05 | 0 | 0.22 | 1.2586 | 3.47 | 1.14 | -0.53 | Tao et al., 2009 | Wheat |
| Acenaphthene | 154.21 | 1.6 | 1.05 | 0 | 0.22 | 1.2586 | 5.31 | 1.14 | -0.38 | Tao et al., 2009 | Wheat |
| Acenaphthene | 154.21 | 1.6 | 1.05 | 0 | 0.22 | 1.2586 | 3.47 | 1.14 | -0.46 | Tao et al., 2009 | Wheat |
| Acenaphthene | 154.21 | 1.6 | 1.05 | 0 | 0.22 | 1.2586 | 6.22 | 1.14 | -0.68 | Tao et al., 2009 | Wheat |
| Acenaphthene | 154.21 | 1.6 | 1.05 | 0 | 0.22 | 1.2586 | 4.81 | 1.14 | -0.31 | Tao et al., 2009 | Wheat |
| Acenaphthene | 154.21 | 1.6 | 1.05 | 0 | 0.22 | 1.2586 | 2.67 | 1.14 | -0.18 | Tao et al., 2009 | Wheat |
| Acenaphthene | 154.21 | 1.6 | 1.05 | 0 | 0.22 | 1.2586 | 4.74 | 1.14 | -0.25 | Tao et al., 2009 | Wheat |
| Acenaphthene | 154.21 | 1.6 | 1.05 | 0 | 0.22 | 1.2586 | 4.16 | 1.14 | -0.39 | Tao et al., 2009 | Wheat |
| Fluorene | 166.22 | 1.59 | 1.061 | 0 | 0.24 | 1.357 | 1.41 | 1.14 | -0.04 | Tao et al., 2009 | Wheat |
| Fluorene | 166.22 | 1.59 | 1.061 | 0 | 0.24 | 1.357 | 4.33 | 1.14 | -0.28 | Tao et al., 2009 | Wheat |
| Fluorene | 166.22 | 1.59 | 1.061 | 0 | 0.24 | 1.357 | 5.71 | 1.14 | -0.55 | Tao et al., 2009 | Wheat |
| Fluorene | 166.22 | 1.59 | 1.061 | 0 | 0.24 | 1.357 | 3.47 | 1.14 | -0.35 | Tao et al., 2009 | Wheat |
| Fluorene | 166.22 | 1.59 | 1.061 | 0 | 0.24 | 1.357 | 5.31 | 1.14 | -0.4 | Tao et al., 2009 | Wheat |
| Fluorene | 166.22 | 1.59 | 1.061 | 0 | 0.24 | 1.357 | 3.47 | 1.14 | -0.48 | Tao et al., 2009 | Wheat |
| Fluorene | 166.22 | 1.59 | 1.061 | 0 | 0.24 | 1.357 | 6.22 | 1.14 | -0.66 | Tao et al., 2009 | Wheat |
| Fluorene | 166.22 | 1.59 | 1.061 | 0 | 0.24 | 1.357 | 4.81 | 1.14 | -0.2 | Tao et al., 2009 | Wheat |
| Fluorene | 166.22 | 1.59 | 1.061 | 0 | 0.24 | 1.357 | 2.67 | 1.14 | -0.12 | Tao et al., 2009 | Wheat |
| Fluorene | 166.22 | 1.59 | 1.061 | 0 | 0.24 | 1.357 | 4.16 | 1.14 | -0.3 | Tao et al., 2009 | Wheat |
| Phenanthrene | 178.23 | 2.06 | 1.29 | 0 | 0.26 | 1.4544 | 5.31 | 1.14 | -0.74 | Tao et al., 2009 | Wheat |
| Phenanthrene | 178.23 | 2.06 | 1.29 | 0 | 0.26 | 1.4544 | 1.41 | 1.14 | -0.16 | Tao et al., 2009 | Wheat |
| Phenanthrene | 178.23 | 2.06 | 1.29 | 0 | 0.26 | 1.4544 | 4.33 | 1.14 | -0.27 | Tao et al., 2009 | Wheat |
| Phenanthrene | 178.23 | 2.06 | 1.29 | 0 | 0.26 | 1.4544 | 2.71 | 1.14 | -0.14 | Tao et al., 2009 | Wheat |
| Phenanthrene | 178.23 | 2.06 | 1.29 | 0 | 0.26 | 1.4544 | 5.71 | 1.14 | -0.8 | Tao et al., 2009 | Wheat |
| Phenanthrene | 178.23 | 2.06 | 1.29 | 0 | 0.26 | 1.4544 | 2.6 | 1.14 | -0.14 | Tao et al., 2009 | Wheat |
| Phenanthrene | 178.23 | 2.06 | 1.29 | 0 | 0.26 | 1.4544 | 3.47 | 1.14 | -0.54 | Tao et al., 2009 | Wheat |
| Phenanthrene | 178.23 | 2.06 | 1.29 | 0 | 0.26 | 1.4544 | 5.31 | 1.14 | -0.56 | Tao et al., 2009 | Wheat |
| Phenanthrene | 178.23 | 2.06 | 1.29 | 0 | 0.26 | 1.4544 | 6.22 | 1.14 | -0.72 | Tao et al., 2009 | Wheat |
| Phenanthrene | 178.23 | 2.06 | 1.29 | 0 | 0.26 | 1.4544 | 4.81 | 1.14 | -0.36 | Tao et al., 2009 | Wheat |
| Phenanthrene | 178.23 | 2.06 | 1.29 | 0 | 0.26 | 1.4544 | 2.67 | 1.14 | -0.22 | Tao et al., 2009 | Wheat |
| Phenanthrene | 178.23 | 2.06 | 1.29 | 0 | 0.26 | 1.4544 | 4.74 | 1.14 | -0.47 | Tao et al., 2009 | Wheat |
| Phenanthrene | 178.23 | 2.06 | 1.29 | 0 | 0.26 | 1.4544 | 4.16 | 1.14 | -0.41 | Tao et al., 2009 | Wheat |
| Anthracene | 178.23 | 2.29 | 1.34 | 0 | 0.28 | 1.4544 | 5.31 | 1.14 | -0.87 | Tao et al., 2009 | Wheat |
| Anthracene | 178.23 | 2.29 | 1.34 | 0 | 0.28 | 1.4544 | 1.41 | 1.14 | -0.22 | Tao et al., 2009 | Wheat |
| Anthracene | 178.23 | 2.29 | 1.34 | 0 | 0.28 | 1.4544 | 2.71 | 1.14 | -0.24 | Tao et al., 2009 | Wheat |
| Anthracene | 178.23 | 2.29 | 1.34 | 0 | 0.28 | 1.4544 | 5.71 | 1.14 | -0.7 | Tao et al., 2009 | Wheat |
| Anthracene | 178.23 | 2.29 | 1.34 | 0 | 0.28 | 1.4544 | 2.6 | 1.14 | -0.51 | Tao et al., 2009 | Wheat |
| Anthracene | 178.23 | 2.29 | 1.34 | 0 | 0.28 | 1.4544 | 3.47 | 1.14 | -0.34 | Tao et al., 2009 | Wheat |
| Anthracene | 178.23 | 2.29 | 1.34 | 0 | 0.28 | 1.4544 | 5.31 | 1.14 | -0.39 | Tao et al., 2009 | Wheat |
| Anthracene | 178.23 | 2.29 | 1.34 | 0 | 0.28 | 1.4544 | 3.47 | 1.14 | -0.95 | Tao et al., 2009 | Wheat |
| Anthracene | 178.23 | 2.29 | 1.34 | 0 | 0.28 | 1.4544 | 6.22 | 1.14 | -0.66 | Tao et al., 2009 | Wheat |
| Anthracene | 178.23 | 2.29 | 1.34 | 0 | 0.28 | 1.4544 | 4.81 | 1.14 | -0.29 | Tao et al., 2009 | Wheat |
| Anthracene | 178.23 | 2.29 | 1.34 | 0 | 0.28 | 1.4544 | 4.74 | 1.14 | -0.35 | Tao et al., 2009 | Wheat |
| Anthracene | 178.23 | 2.29 | 1.34 | 0 | 0.28 | 1.4544 | 4.16 | 1.14 | -0.29 | Tao et al., 2009 | Wheat |
| Fluoranthene | 202.25 | 2.377 | 1.55 | 0 | 0.24 | 1.585 | 1.41 | 1.14 | 0.01 | Tao et al., 2009 | Wheat |
| Fluoranthene | 202.25 | 2.377 | 1.55 | 0 | 0.24 | 1.585 | 4.33 | 1.14 | -0.43 | Tao et al., 2009 | Wheat |
| Fluoranthene | 202.25 | 2.377 | 1.55 | 0 | 0.24 | 1.585 | 5.71 | 1.14 | -0.45 | Tao et al., 2009 | Wheat |
| Fluoranthene | 202.25 | 2.377 | 1.55 | 0 | 0.24 | 1.585 | 3.47 | 1.14 | -0.26 | Tao et al., 2009 | Wheat |
| Fluoranthene | 202.25 | 2.377 | 1.55 | 0 | 0.24 | 1.585 | 5.31 | 1.14 | -0.45 | Tao et al., 2009 | Wheat |
| Pyrene | 202.25 | 2.81 | 1.71 | 0 | 0.28 | 1.5846 | 1.41 | 1.14 | -0.13 | Tao et al., 2009 | Wheat |
| Pyrene | 202.25 | 2.81 | 1.71 | 0 | 0.28 | 1.5846 | 4.33 | 1.14 | -0.5 | Tao et al., 2009 | Wheat |
| Pyrene | 202.25 | 2.81 | 1.71 | 0 | 0.28 | 1.5846 | 5.71 | 1.14 | -0.53 | Tao et al., 2009 | Wheat |
| Pyrene | 202.25 | 2.81 | 1.71 | 0 | 0.28 | 1.5846 | 3.47 | 1.14 | -0.28 | Tao et al., 2009 | Wheat |
| Pyrene | 202.25 | 2.81 | 1.71 | 0 | 0.28 | 1.5846 | 5.31 | 1.14 | -0.6 | Tao et al., 2009 | Wheat |
| Pyrene | 202.25 | 2.81 | 1.71 | 0 | 0.28 | 1.5846 | 6.22 | 1.14 | -0.53 | Tao et al., 2009 | Wheat |
| Benzo[a]anthracene | 228.3 | 2.99 | 1.7 | 0 | 0.35 | 1.8234 | 1.41 | 1.14 | 0.11 | Tao et al., 2009 | Wheat |
| Benzo[a]anthracene | 228.3 | 2.99 | 1.7 | 0 | 0.35 | 1.8234 | 4.33 | 1.14 | -0.44 | Tao et al., 2009 | Wheat |
| Benzo[a]anthracene | 228.3 | 2.99 | 1.7 | 0 | 0.35 | 1.8234 | 5.31 | 1.14 | -0.72 | Tao et al., 2009 | Wheat |
| Benzo[a]anthracene | 228.3 | 2.99 | 1.7 | 0 | 0.35 | 1.8234 | 3.47 | 1.14 | -0.35 | Tao et al., 2009 | Wheat |
| Chrysene | 228.3 | 3.03 | 1.73 | 0 | 0.33 | 1.8234 | 5.31 | 1.14 | -1.23 | Tao et al., 2009 | Wheat |
| Chrysene | 228.3 | 3.03 | 1.73 | 0 | 0.33 | 1.8234 | 1.41 | 1.14 | 0.08 | Tao et al., 2009 | Wheat |
| Chrysene | 228.3 | 3.03 | 1.73 | 0 | 0.33 | 1.8234 | 5.71 | 1.14 | -0.52 | Tao et al., 2009 | Wheat |
| Chrysene | 228.3 | 3.03 | 1.73 | 0 | 0.33 | 1.8234 | 3.47 | 1.14 | -0.33 | Tao et al., 2009 | Wheat |
| benzo[b]fluoranthene | 252.3 | 3.19 | 1.82 | 0 | 0.4 | 1.9536 | 3.47 | 1.14 | -0.81 | Tao et al., 2009 | Wheat |
| benzo[b]fluoranthene | 252.3 | 3.19 | 1.82 | 0 | 0.4 | 1.9536 | 6.22 | 1.14 | -0.98 | Tao et al., 2009 | Wheat |
| benzo[b]fluoranthene | 252.3 | 3.19 | 1.82 | 0 | 0.4 | 1.9536 | 4.81 | 1.14 | -0.76 | Tao et al., 2009 | Wheat |
| benzo[b]fluoranthene | 252.3 | 3.19 | 1.82 | 0 | 0.4 | 1.9536 | 2.67 | 1.14 | -0.2 | Tao et al., 2009 | Wheat |
| benzo[b]fluoranthene | 252.3 | 3.19 | 1.82 | 0 | 0.4 | 1.9536 | 4.16 | 1.14 | -0.66 | Tao et al., 2009 | Wheat |
| benzo[k]fluoranthene | 252.3 | 3.19 | 1.91 | 0 | 0.33 | 1.9536 | 4.33 | 1.14 | -1.39 | Tao et al., 2009 | Wheat |
| benzo[k]fluoranthene | 252.3 | 3.19 | 1.91 | 0 | 0.33 | 1.9536 | 2.71 | 1.14 | -0.71 | Tao et al., 2009 | Wheat |
| benzo[k]fluoranthene | 252.3 | 3.19 | 1.91 | 0 | 0.33 | 1.9536 | 5.71 | 1.14 | -1.04 | Tao et al., 2009 | Wheat |
| benzo[k]fluoranthene | 252.3 | 3.19 | 1.91 | 0 | 0.33 | 1.9536 | 3.47 | 1.14 | -1 | Tao et al., 2009 | Wheat |
| benzo[k]fluoranthene | 252.3 | 3.19 | 1.91 | 0 | 0.33 | 1.9536 | 5.31 | 1.14 | -1.33 | Tao et al., 2009 | Wheat |
| benzo[k]fluoranthene | 252.3 | 3.19 | 1.91 | 0 | 0.33 | 1.9536 | 3.47 | 1.14 | -0.82 | Tao et al., 2009 | Wheat |
| benzo[k]fluoranthene | 252.3 | 3.19 | 1.91 | 0 | 0.33 | 1.9536 | 6.22 | 1.14 | -1.23 | Tao et al., 2009 | Wheat |
| benzo[k]fluoranthene | 252.3 | 3.19 | 1.91 | 0 | 0.33 | 1.9536 | 4.74 | 1.14 | -1.05 | Tao et al., 2009 | Wheat |
| Benzo[a]pyrene | 252.3 | 3.63 | 1.98 | 0 | 0.44 | 1.9536 | 5.31 | 1.14 | -1.58 | Tao et al., 2009 | Wheat |
| Benzo[a]pyrene | 252.3 | 3.63 | 1.98 | 0 | 0.44 | 1.9536 | 4.33 | 1.14 | -1.51 | Tao et al., 2009 | Wheat |
| Benzo[a]pyrene | 252.3 | 3.63 | 1.98 | 0 | 0.44 | 1.9536 | 5.71 | 1.14 | -1.25 | Tao et al., 2009 | Wheat |
| Benzo[a]pyrene | 252.3 | 3.63 | 1.98 | 0 | 0.44 | 1.9536 | 3.47 | 1.14 | -0.98 | Tao et al., 2009 | Wheat |
| Benzo[a]pyrene | 252.3 | 3.63 | 1.98 | 0 | 0.44 | 1.9536 | 6.22 | 1.14 | -1.05 | Tao et al., 2009 | Wheat |
| Dibenzo[a,h]anthracene | 278.3 | 4 | 2.04 | 0 | 0.44 | 2.1924 | 4.33 | 1.14 | -1.49 | Tao et al., 2009 | Wheat |
| Dibenzo[a,h]anthracene | 278.3 | 4 | 2.04 | 0 | 0.44 | 2.1924 | 2.71 | 1.14 | -1.17 | Tao et al., 2009 | Wheat |
| Dibenzo[a,h]anthracene | 278.3 | 4 | 2.04 | 0 | 0.44 | 2.1924 | 2.6 | 1.14 | -1.39 | Tao et al., 2009 | Wheat |
| Dibenzo[a,h]anthracene | 278.3 | 4 | 2.04 | 0 | 0.44 | 2.1924 | 3.47 | 1.14 | -1.22 | Tao et al., 2009 | Wheat |
| Dibenzo[a,h]anthracene | 278.3 | 4 | 2.04 | 0 | 0.44 | 2.1924 | 5.31 | 1.14 | -1.55 | Tao et al., 2009 | Wheat |
| Dibenzo[a,h]anthracene | 278.3 | 4 | 2.04 | 0 | 0.44 | 2.1924 | 3.47 | 1.14 | -1.1 | Tao et al., 2009 | Wheat |
| Benzo[g,h,i]perylene | 276.3 | 4.07 | 1.9 | 0 | 0.45 | 2.0838 | 1.41 | 1.14 | -1.22 | Tao et al., 2009 | Wheat |
| Benzo[g,h,i]perylene | 276.3 | 4.07 | 1.9 | 0 | 0.45 | 2.0838 | 2.71 | 1.14 | -0.99 | Tao et al., 2009 | Wheat |
| Benzo[g,h,i]perylene | 276.3 | 4.07 | 1.9 | 0 | 0.45 | 2.0838 | 5.71 | 1.14 | -1.25 | Tao et al., 2009 | Wheat |
| Benzo[g,h,i]perylene | 276.3 | 4.07 | 1.9 | 0 | 0.45 | 2.0838 | 2.6 | 1.14 | -1.36 | Tao et al., 2009 | Wheat |
| Benzo[g,h,i]perylene | 276.3 | 4.07 | 1.9 | 0 | 0.45 | 2.0838 | 5.31 | 1.14 | -1.65 | Tao et al., 2009 | Wheat |
| Arazine | 215.68 | 1.22 | 1.29 | 0.17 | 1.01 | 1.6196 | 3.55 | 1 | 0.08 | Trapp et al., 1990 | Barely |
| 1,2,4-Trichlorobenzene | 181.4 | 0.98 | 0.81 | 0 | 0 | 1.0836 | 3.55 | 1 | 0.03 | Trapp et al., 1990 | Barely |
| 1,2,3,5-Tetrachlorobenzene | 215.9 | 1.16 | 0.85 | 0 | 0 | 1.206 | 3.55 | 1 | 0.23 | Trapp et al., 1990 | Barely |
| Dieldrin | 380.9 | 2.08 | 0.85 | 0 | 0.56 | 1.9626 | 3.55 | 1 | -0.26 | Trapp et al., 1990 | Barely |
| Hexachlorobenzene | 284.8 | 1.49 | 0.99 | 0 | 0 | 1.4508 | 3.55 | 1 | 0.07 | Trapp et al., 1990 | Barely |
| 2,4,6,2',4'-PCB | 326.4 | 2.04 | 1.61 | 0 | 0.13 | 1.9362 | 3.55 | 1 | 0.07 | Trapp et al., 1990 | Barely |
| DDT | 354.5 | 1.81 | 1.76 | 0 | 0.16 | 2.218 | 3.55 | 1 | -0.48 | Trapp et al., 1990 | Barely |
| Phenanthrene | 178.23 | 2.06 | 1.29 | 0 | 0.26 | 1.4544 | 2 | 0.24 | -0.49 | Kipopoulou et al., 1999 | Carrot |
| Anthracene | 178.23 | 2.29 | 1.34 | 0 | 0.28 | 1.4544 | 2 | 0.24 | -0.85 | Kipopoulou et al., 1999 | Carrot |
| Fluoranthene | 202.25 | 2.377 | 1.55 | 0 | 0.24 | 1.585 | 2 | 0.24 | -0.95 | Kipopoulou et al., 1999 | Carrot |
| Pyrene | 202.25 | 2.81 | 1.71 | 0 | 0.28 | 1.5846 | 2 | 0.24 | -0.85 | Kipopoulou et al., 1999 | Carrot |
| Benzo[a]anthracene | 228.3 | 2.99 | 1.7 | 0 | 0.35 | 1.8234 | 2 | 0.24 | -1.77 | Kipopoulou et al., 1999 | Carrot |
| Chrysene | 228.3 | 3.03 | 1.73 | 0 | 0.33 | 1.8234 | 2 | 0.24 | -1.64 | Kipopoulou et al., 1999 | Carrot |
| Benzo[e]pyrene | 252.3 | 3.63 | 1.96 | 0 | 0.35 | 1.9536 | 2 | 0.24 | -1.74 | Kipopoulou et al., 1999 | Carrot |
| Benzo[b]fluoranthene | 252.3 | 3.19 | 1.82 | 0 | 0.4 | 1.9536 | 2 | 0.24 | -1.92 | Kipopoulou et al., 1999 | Carrot |
| Benzo[k]fluoranthene | 252.3 | 3.19 | 1.91 | 0 | 0.33 | 1.9536 | 2 | 0.24 | -1.85 | Kipopoulou et al., 1999 | Carrot |
| Benzo[a]pyrene | 252.3 | 3.63 | 1.98 | 0 | 0.44 | 1.9536 | 2 | 0.24 | -1.72 | Kipopoulou et al., 1999 | Carrot |
| Dibenz-[a,h]anthracene | 278.3 | 4 | 2.04 | 0 | 0.44 | 2.1924 | 2 | 0.24 | -1.7 | Kipopoulou et al., 1999 | Carrot |
| Benz[phi]perylene | 276.3 | 4.07 | 1.9 | 0 | 0.45 | 2.0838 | 2 | 0.24 | -1.89 | Kipopoulou et al., 1999 | Carrot |
| Indeno[1,2,3-cd]pyrene | 276.3 | 3.61 | 1.93 | 0 | 0.42 | 2.0838 | 2 | 0.24 | -1.8 | Kipopoulou et al., 1999 | Carrot |
| Galaxolide | 258.4 | 1.09 | 1.15 | 0 | 0.63 | 2.2487 | 1.55 | 0.24 | -1.05 | Macherius et al., 2012 | Carrot |
| Galaxolide | 258.4 | 1.09 | 1.15 | 0 | 0.63 | 2.2487 | 1.55 | 1 | -1.08 | Macherius et al., 2012 | Barely |
| Tonalide | 258.4 | 1.05 | 1.06 | 0 | 0.68 | 2.3143 | 1.55 | 0.24 | -1.3 | Macherius et al., 2012 | Carrot |
| Tonalide | 258.4 | 1.05 | 1.06 | 0 | 0.68 | 2.3143 | 1.55 | 1 | -0.83 | Macherius et al., 2012 | Barely |
| Triclosan | 289.5 | 1.73 | 1.55 | 0.47 | 0.45 | 1.8088 | 13.8 | 0.1 | -1.03 | Pannu et al., 2012 | Radish |
| Triclosan | 289.5 | 1.73 | 1.55 | 0.47 | 0.45 | 1.8088 | 4.1 | 0.1 | -0.8 | Prosser et al., 2014 | Radish |
| Triclosan | 289.5 | 1.73 | 1.55 | 0.47 | 0.45 | 1.8088 | 3.9 | 0.24 | -0.62 | Prosser et al., 2014 | Carrot |
| Trimethoprim | 290.32 | 1.89 | 2.5 | 0.21 | 1.69 | 2.1813 | 0.69 | 0.24 | -1.1 | Boxall et al., 2006 | Carrot |
| Carbamazepine | 236.27 | 2.15 | 1.9 | 0.5 | 1.15 | 1.8106 | 1.72 | 0.1 | 0.92 | Carter et al., 2014 | Radish |
| alpha-endosulfan | 406.9 | 2.23 | 0.94 | 0 | 1.03 | 2.0819 | 8.8 | 0.1 | -0.6127882 | GONZALEZ et al., 2003 | leek |
| endosulfan sulfate | 422.9 | 2.16 | 1.57 | 0 | 1.19 | 2.1406 | 8.8 | 0.1 | 0.377451963 | GONZALEZ et al., 2003 | leek |
| dieldrin | 380.9 | 2.09 | 1.57 | 0 | 0.75 | 2.0065 | 8.8 | 0.1 | -0.663940722 | GONZALEZ et al., 2003 | leek |
| heptachlor | 373.3 | 2.08 | 0.85 | 0 | 0.56 | 1.9626 | 8.8 | 0.1 | 0.218299126 | GONZALEZ et al., 2003 | leek |
| heptachlor epoxide | 389.3 | 2.22 | 1.11 | 0 | 0.53 | 1.9557 | 8.8 | 0.1 | -0.868060705 | GONZALEZ et al., 2003 | leek |
| Acetamiprid | 222.67 | 1.4 | 1.57 | 0.05 | 1.21 | 1.6726 | 3.05 | 0.53 | -0.175729196 | Wang et.al., 2021 | Maize |
| Azoxystrobin | 403.4 | 2.59 | 2.01 | 0 | 2.3 | 2.9165 | 3.05 | 0.53 | -0.137461857 | Wang et.al., 2021 | Maize |
| Tebuconazole | 307.82 | 1.54 | 1.45 | 0.24 | 1.44 | 2.4113 | 3.05 | 0.53 | -0.07773118 | Wang et.al., 2021 | Maize |

Table S2: Molecular properties of chemicals calculated from RdKit package

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Compounds | NOCount | NHOHCount | NumHAcceptors | NumHDonors | Num\_Aro\_rings | tpsa | Num\_sat\_rings |
| Penconazole | 3 | 3 | 3 | 3 | 3 | 30.71 | 0 |
| Penconazole | 3 | 3 | 3 | 3 | 3 | 30.71 | 0 |
| Penconazole | 3 | 3 | 3 | 3 | 3 | 30.71 | 0 |
| Penconazole | 3 | 3 | 3 | 3 | 3 | 30.71 | 0 |
| Penconazole | 3 | 3 | 3 | 3 | 3 | 30.71 | 0 |
| Aldrin  | 0 | 0 | 0 | 0 | 0 | 0 | 2 |
| Aldrin  | 0 | 0 | 0 | 0 | 0 | 0 | 2 |
| Dieldrin | 1 | 1 | 1 | 1 | 1 | 12.53 | 4 |
| Dieldrin | 1 | 1 | 1 | 1 | 1 | 12.53 | 4 |
| Dieldrin | 1 | 1 | 1 | 1 | 1 | 12.53 | 4 |
| Dieldrin | 1 | 1 | 1 | 1 | 1 | 12.53 | 4 |
| Dieldrin | 1 | 1 | 1 | 1 | 1 | 12.53 | 4 |
| Dieldrin | 1 | 1 | 1 | 1 | 1 | 12.53 | 4 |
| m-DCB (1,3-DCB) | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| m-DCB (1,3-DCB) | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| m-DCB (1,3-DCB) | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| m-DCB (1,3-DCB) | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| m-DCB (1,3-DCB) | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| m-DCB (1,3-DCB) | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| p-DCB (1,4-DCB) | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| p-DCB (1,4-DCB) | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| p-DCB (1,4-DCB) | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| o-DCB (1,2-DCB) | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| o-DCB (1,2-DCB) | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| o-DCB (1,2-DCB) | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 1,2,4-TCB | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 1,2,4-TCB | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 1,2,4-TCB | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 1,2,4-TCB | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 1,2,4-TCB | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 1,2,4-TCB | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 1,2,4-TCB | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 1,2,4-TCB | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Fluorene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Phenanthrene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Phenanthrene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Anthracene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Anthracene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Fluoranthene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Benzo[a]pyrene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Di(2-ethylhexyl) phthalate | 4 | 4 | 4 | 4 | 4 | 52.6 | 0 |
| Di(2-ethylhexyl) phthalate | 4 | 4 | 4 | 4 | 4 | 52.6 | 0 |
| Phenanthrene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Phenanthrene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Pyrene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| HCB | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| o,p'-DDE | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| p,p'-DDE | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| o,p'-DDD | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| p,p'-DDD | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| o,p'-DDT | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| p,p'-DDT | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| PCB 101 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| PCB 153 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| PCB 138 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| PCB 180 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| BDE-100 | 1 | 1 | 1 | 1 | 1 | 9.23 | 0 |
| BDE-100 | 1 | 1 | 1 | 1 | 1 | 9.23 | 0 |
| BDE-100 | 1 | 1 | 1 | 1 | 1 | 9.23 | 0 |
| BDE-100 | 1 | 1 | 1 | 1 | 1 | 9.23 | 0 |
| BDE-100 | 1 | 1 | 1 | 1 | 1 | 9.23 | 0 |
| BDE-100 | 1 | 1 | 1 | 1 | 1 | 9.23 | 0 |
| BDE-153 | 1 | 1 | 1 | 1 | 1 | 9.23 | 0 |
| BDE-153 | 1 | 1 | 1 | 1 | 1 | 9.23 | 0 |
| BDE-153 | 1 | 1 | 1 | 1 | 1 | 9.23 | 0 |
| BDE-153 | 1 | 1 | 1 | 1 | 1 | 9.23 | 0 |
| BDE-153 | 1 | 1 | 1 | 1 | 1 | 9.23 | 0 |
| BDE-154 | 1 | 1 | 1 | 1 | 1 | 9.23 | 0 |
| BDE-154 | 1 | 1 | 1 | 1 | 1 | 9.23 | 0 |
| BDE-154 | 1 | 1 | 1 | 1 | 1 | 9.23 | 0 |
| BDE-154 | 1 | 1 | 1 | 1 | 1 | 9.23 | 0 |
| BDE-154 | 1 | 1 | 1 | 1 | 1 | 9.23 | 0 |
| BDE-154 | 1 | 1 | 1 | 1 | 1 | 9.23 | 0 |
| BDE-183 | 1 | 1 | 1 | 1 | 1 | 9.23 | 0 |
| BDE-183 | 1 | 1 | 1 | 1 | 1 | 9.23 | 0 |
| BDE-183 | 1 | 1 | 1 | 1 | 1 | 9.23 | 0 |
| BDE-183 | 1 | 1 | 1 | 1 | 1 | 9.23 | 0 |
| BDE-183 | 1 | 1 | 1 | 1 | 1 | 9.23 | 0 |
| BDE-183 | 1 | 1 | 1 | 1 | 1 | 9.23 | 0 |
| BDE-28 | 1 | 1 | 1 | 1 | 1 | 9.23 | 0 |
| BDE-28 | 1 | 1 | 1 | 1 | 1 | 9.23 | 0 |
| BDE-47 | 1 | 1 | 1 | 1 | 1 | 9.23 | 0 |
| BDE-47 | 1 | 1 | 1 | 1 | 1 | 9.23 | 0 |
| BDE-47 | 1 | 1 | 1 | 1 | 1 | 9.23 | 0 |
| BDE-47 | 1 | 1 | 1 | 1 | 1 | 9.23 | 0 |
| BDE-47 | 1 | 1 | 1 | 1 | 1 | 9.23 | 0 |
| BDE-47 | 1 | 1 | 1 | 1 | 1 | 9.23 | 0 |
| BDE-99 | 1 | 1 | 1 | 1 | 1 | 9.23 | 0 |
| BDE-99 | 1 | 1 | 1 | 1 | 1 | 9.23 | 0 |
| BDE-99 | 1 | 1 | 1 | 1 | 1 | 9.23 | 0 |
| BDE-99 | 1 | 1 | 1 | 1 | 1 | 9.23 | 0 |
| BDE-99 | 1 | 1 | 1 | 1 | 1 | 9.23 | 0 |
| BDE-99 | 1 | 1 | 1 | 1 | 1 | 9.23 | 0 |
| Dieldrin | 1 | 1 | 1 | 1 | 1 | 12.53 | 4 |
| Dieldrin | 1 | 1 | 1 | 1 | 1 | 12.53 | 4 |
| Dieldrin | 1 | 1 | 1 | 1 | 1 | 12.53 | 4 |
| Dieldrin | 1 | 1 | 1 | 1 | 1 | 12.53 | 4 |
| Dieldrin | 1 | 1 | 1 | 1 | 1 | 12.53 | 4 |
| Dieldrin | 1 | 1 | 1 | 1 | 1 | 12.53 | 4 |
| 1,4-DCB | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 1,2,4-TCB | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 1,2,3,5-TeCB | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Pentachlorobeneze | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Hexachlorobenze | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Naphthalene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Naphthalene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Naphthalene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Naphthalene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Naphthalene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Naphthalene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Naphthalene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Naphthalene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Naphthalene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Naphthalene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Acenaphthene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Acenaphthene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Acenaphthene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Acenaphthene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Acenaphthene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Acenaphthene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Acenaphthene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Acenaphthene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Acenaphthene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Acenaphthene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Acenaphthene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Acenaphthene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Fluorene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Fluorene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Fluorene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Fluorene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Fluorene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Fluorene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Fluorene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Fluorene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Fluorene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Fluorene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Phenanthrene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Phenanthrene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Phenanthrene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Phenanthrene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Phenanthrene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Phenanthrene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Phenanthrene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Phenanthrene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Phenanthrene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Phenanthrene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Phenanthrene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Phenanthrene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Phenanthrene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Anthracene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Anthracene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Anthracene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Anthracene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Anthracene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Anthracene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Anthracene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Anthracene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Anthracene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Anthracene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Anthracene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Anthracene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Fluoranthene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Fluoranthene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Fluoranthene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Fluoranthene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Fluoranthene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Pyrene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Pyrene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Pyrene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Pyrene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Pyrene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Pyrene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Benzo[a]anthracene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Benzo[a]anthracene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Benzo[a]anthracene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Benzo[a]anthracene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Chrysene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Chrysene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Chrysene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Chrysene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| benzo[b]fluoranthene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| benzo[b]fluoranthene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| benzo[b]fluoranthene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| benzo[b]fluoranthene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| benzo[b]fluoranthene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| benzo[k]fluoranthene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| benzo[k]fluoranthene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| benzo[k]fluoranthene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| benzo[k]fluoranthene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| benzo[k]fluoranthene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| benzo[k]fluoranthene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| benzo[k]fluoranthene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| benzo[k]fluoranthene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Benzo[a]pyrene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Benzo[a]pyrene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Benzo[a]pyrene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Benzo[a]pyrene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Benzo[a]pyrene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Dibenzo[a,h]anthracene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Dibenzo[a,h]anthracene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Dibenzo[a,h]anthracene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Dibenzo[a,h]anthracene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Dibenzo[a,h]anthracene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Dibenzo[a,h]anthracene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Benzo[g,h,i]perylene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Benzo[g,h,i]perylene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Benzo[g,h,i]perylene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Benzo[g,h,i]perylene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Benzo[g,h,i]perylene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Arazine | 5 | 5 | 5 | 5 | 5 | 62.73 | 0 |
| 1,2,4-Trichlorobenzene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 1,2,3,5-Tetrachlorobenzene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Dieldrin | 1 | 1 | 1 | 1 | 1 | 12.53 | 4 |
| Hexachlorobenzene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 2,4,6,2',4'-PCB | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| DDT | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Phenanthrene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Anthracene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Fluoranthene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Pyrene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Benzo[a]anthracene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Chrysene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Benzo[e]pyrene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Benzo[b]fluoranthene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Benzo[k]fluoranthene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Benzo[a]pyrene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Dibenz-[a,h]anthracene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Benz[phi]perylene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Indeno[1,2,3-cd]pyrene | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| Galaxolide | 1 | 1 | 1 | 1 | 1 | 9.23 | 0 |
| Galaxolide | 1 | 1 | 1 | 1 | 1 | 9.23 | 0 |
| Tonalide | 1 | 1 | 1 | 1 | 1 | 17.07 | 0 |
| Tonalide | 1 | 1 | 1 | 1 | 1 | 17.07 | 0 |
| Triclosan | 2 | 2 | 2 | 2 | 2 | 29.46 | 0 |
| Triclosan | 2 | 2 | 2 | 2 | 2 | 29.46 | 0 |
| Triclosan | 2 | 2 | 2 | 2 | 2 | 29.46 | 0 |
| Trimethoprim | 7 | 7 | 7 | 7 | 7 | 105.51 | 0 |
| Carbamazepine | 3 | 3 | 3 | 3 | 3 | 46.33 | 0 |
| alpha-endosulfan | 3 | 3 | 3 | 3 | 3 | 35.53 | 2 |
| endosulfan sulfate | 4 | 4 | 4 | 4 | 4 | 52.6 | 2 |
| dieldrin | 1 | 1 | 1 | 1 | 1 | 12.53 | 4 |
| heptachlor | 0 | 0 | 0 | 0 | 0 | 0 | 1 |
| heptachlor epoxide | 1 | 1 | 1 | 1 | 1 | 12.53 | 3 |
| Acetamiprid | 4 | 4 | 4 | 4 | 4 | 52.28 | 0 |
| Azoxystrobin | 8 | 8 | 8 | 8 | 8 | 103.56 | 0 |
| Tebuconazole | 4 | 4 | 4 | 4 | 4 | 50.94 | 0 |

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