SUPPLEMENTARY MATERIAL

Designing Quantitative Structure Activity Relationships to Predict Specific Toxic Endpoints for Polybrominated Diphenyl Ethers in Mammalian Cells

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Table S1. Relevant ANOVA statistics for cell viability studies

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Endpoint | Cell Viability | | | | | |
| Comparison | Control and Sol. Control | | | Sol. Control and treatments | | |
| Chem ↓ Stats → | N | F - stat | p-value | N | F - stat | p-value |
| PBDE - 28 | 8 | 2.878773 | 0.111865 | 16 | 56.81516 | 3.27E-25 |
| PBDE - 47 | 8 | 0.008018 | 0.92992 | 16 | 11.04162 | 3.79E-08 |
| PBDE - 99 | 8 | 0.935019 | 0.349971 | 16 | 5.657927 | 0.000157 |
| BDE - 100 | 8 | 0.007815 | 0.930809 | 16 | 4.045398 | 0.002483 |
| PBDE - 153 | 8 | 0.436464 | 0.519558 | 16 | 1.330426 | 0.001859 |
| PBDE - 183 | 8 | 0.022222 | 0.883624 | 16 | 15.41681 | 1.15E-10 |
| PBDE - 209 | 8 | 1.382558 | 0.259275 | 16 | 6.517038 | 3.77E-05 |
| 3-OH-BDE-47 | 8 | 1.684044 | 0.215363 | 16 | 8.710034 | 1.17E-06 |
| 5-OH-BDE-47 | 8 | 0.649907 | 0.433627 | 16 | 14.44014 | 3.92E-10 |
| 6-OH-BDE-47 | 8 | 2.091512 | 0.170135 | 16 | 50.71747 | 1.11E-23 |

Table S2. Relevant ANOVA statistics for apoptosis studies

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Endpoint | Apoptosis | | | | | |
| Comparison | Control and Sol. Control | | | Sol. Control and treatments | | |
| Chem ↓ Stats → | N | F - stat | p-value | N | F - stat | p-value |
| PBDE - 28 | 8 | 5.542826 | 0.063685 | 16 | 5.156622 | 0.000366 |
| PBDE - 47 | 8 | 0.754162 | 0.399804 | 16 | 1.208202 | 0.003126 |
| PBDE - 99 | 8 | 0.938715 | 0.34905 | 16 | 2.90064 | 0.018408 |
| BDE - 100 | 8 | 0.084722 | 0.775265 | 16 | 0.595527 | 0.007034 |
| PBDE - 153 | 8 | 0.174383 | 0.682579 | 16 | 2.451075 | 0.040277 |
| PBDE - 183 | 8 | 1.472954 | 0.244959 | 16 | 2.255287 | 0.056451 |
| PBDE - 209 | 8 | 0.027075 | 0.871655 | 16 | 3.888296 | 0.003266 |
| 3-OH-BDE-47 | 8 | 0.286111 | 0.601116 | 16 | 0.805585 | 0.548946 |
| 5-OH-BDE-47 | 8 | 1.737766 | 0.208584 | 16 | 42.07957 | 2.94E-21 |
| 6-OH-BDE-47 | 8 | 4.806187 | 0.055755 | 16 | 73.56653 | 7.56E-29 |

|  |  |
| --- | --- |
| Table S3**.** Log Kow values for specific PBDE congeners (46) | |
| Chemical | Log Kow |
| PBDE-28 | 5.94± 0.15 |
| PBDE-47 | 6.81± 0.08 |
| PBDE-99 | 7.32± 0.14 |
| PBDE-100 | 7.24± 0.16 |
| PBDE-153 | 7.90± 0.14 |
| PBDE-183 | 8.27± 0.26 |

Table S4 : Two – dimensional structures of PBDE congeners

|  |  |
| --- | --- |
| PBDE Congener | Structure |
| PBDE - 28 | **C:\Users\Swati\Documents\LabMain\Publication SAR & QSAR in Env. Research\Submission\Final Submission\For revision\2D PBDE structures\New\PBDE 28.tif** |
| PBDE - 47 | C:\Users\Swati\Documents\LabMain\Publication SAR & QSAR in Env. Research\Submission\Final Submission\For revision\2D PBDE structures\New\PBDE 47.tif |
| PBDE- 99 | C:\Users\Swati\Documents\LabMain\Publication SAR & QSAR in Env. Research\Submission\Final Submission\For revision\2D PBDE structures\New\PBDE 99.tif |
| PBDE - 100 | C:\Users\Swati\Documents\LabMain\Publication SAR & QSAR in Env. Research\Submission\Final Submission\For revision\2D PBDE structures\New\PBDE 100.tif |
| PBDE - 153 | C:\Users\Swati\Documents\LabMain\Publication SAR & QSAR in Env. Research\Submission\Final Submission\For revision\2D PBDE structures\New\PBDE 153.tif |
| PBDE – 183 | C:\Users\Swati\Documents\LabMain\Publication SAR & QSAR in Env. Research\Submission\Final Submission\For revision\2D PBDE structures\New\PBDE 183.tif |
| PBDE - 209 | C:\Users\Swati\Documents\LabMain\Publication SAR & QSAR in Env. Research\Submission\Final Submission\For revision\2D PBDE structures\New\PBDE 209 .tif |
| 3-OH- BDE- 47 | C:\Users\Swati\Documents\LabMain\Publication SAR & QSAR in Env. Research\Submission\Final Submission\For revision\2D PBDE structures\New\3 - OH - PBDE 47.tif |
| 5-OH- BDE- 47 | C:\Users\Swati\Documents\LabMain\Publication SAR & QSAR in Env. Research\Submission\Final Submission\For revision\2D PBDE structures\New\5 - OH - PBDE 47.tif |
| 6-OH-BDE- 47 | C:\Users\Swati\Documents\LabMain\Publication SAR & QSAR in Env. Research\Submission\Final Submission\For revision\2D PBDE structures\New\6 - OH - PBDE 47.tif |

Table S5 : Three – dimensional structures of PBDE congeners

|  |  |
| --- | --- |
| PBDE Congener | Structure |
| PBDE - 28 |  |
| PBDE - 47 |  |
| PBDE- 99 |  |
| PBDE - 100 |  |

|  |  |
| --- | --- |
| PBDE – 153 |  |
| PBDE – 183 |  |
| PBDE – 209 |  |
| 3-OH- BDE- 47 |  |
| 5-OH- BDE- 47 |  |
| 6-OH-BDE- 47 |  |

Table S6. Calculated values for descriptors used in QSAR equations

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Chemical | Atom | Id. # | ALogP\_AtomMRScore | Gasteiger\_Charges | VSA\_AtomicAreas | VSA\_PartialCharge | Kappa\_3 |
| PBDE-28 | C1  C1  C2  C3  C4  C5  O6  C7  C8  C9  C10  C11  C12  Br13  Br14  Br15  H1  H2  H3  H4  H5  H6  H7 | 0  1  2  3  4  5  6  7  8  9  10  11  12  13  14  15  1  2  3  4  5  6  7 | 8.20653.75933.44913.75938.20653.44913.44913.75931.35023.75933.44913.44913.7593  8.2065  3.4491  3.4491  0.8939  0.8939  0.8939  0.8939  0.8939  0.8939  0.8939 | -4.79e-002 4.94e-002 -3.11e-002 1.88e-002 -5.08e-002 -4.53e-002 -2.9e-002 9.62e-002 -0.3093 8.21e-002 -3.02e-002 -4.54e-002 1.76e-002 -5.09e-002 -4.54e-002 -3.02e-002 6.47e-002 6.35e-002 6.51e-002 6.5e-002 6.35e-002 6.35e-002 6.61e-002 | 42.496 4.365 9.564 4.365 42.496 9.564 9.564 7.867 8.689 7.867 9.564 9.564 4.365 42.496 9.564 9.564 7.657 7.657 7.657 7.657 7.657 7.657 7.657 | 8.689 0 0 0 0 84.992 109.444 13.097 69.337 0 0 0 0 0 | 3.49519 |

Table S6continued

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Chemical | | | | | Atom | | | | | Id. # | | | | | ALogP\_AtomMRScore | | | | | | | Gasteiger\_Charges | | | | | | | | | | | VSA\_AtomicAreas | | | | | | | | | | | VSA\_PartialCharge | | | | | | | | | | | | | Kappa\_3 | | | |
| BDE-47 | | | | | C1  C1  C2  C3  C4  C5  Br6  Br7  O8  C9  C10  C11  C12  C13  C14  Br15  Br16  H1  H2  H3  H4  H5  H6 | | | | | 0  1  2  3  4  5  6  7  8  9  10  11  12  13  14  15  16  1  2  3  4  5  6 | | | | | 3.44913.44913.75933.75933.44913.75938.20658.20651.35023.75933.7593  3.4491  3.7593  3.4491  3.4491  8.2065  8.2065  0.8939  0.8939  0.8939  0.8939  0.8939  0.8939 | | | | | | | -4.53e-002 -2.9e-002 9.63e-002 4.94e-002 -3.11e-002 1.88e-002 -5.08e-002 -4.79e-002 -0.3081 9.63e-002 4.94e-002 -3.11e-002 1.88e-002 -4.53e-002 -2.9e-002 -5.08e-002 -4.79e-002 6.35e-002 6.51e-002 6.47e-002 6.47e-002 6.35e-002 6.58000 | | | | | | | | | | | 9.564 9.564 7.867 4.365 9.564 4.365 42.496 42.496 8.689 7.867 4.365 9.564 4.365 9.564 9.564 42.496 42.496 7.657 7.657 7.657 7.657 7.657 7.657 | | | | | | | | | | | 8.689 0 0 0 0 84.992 142.376 17.462 61.679 0 0 0 0 0 | | | | | | | | | | | | | 3.48444 | | | |
|  | | | | |  | | | | |  | | | | |  | | | | | | |  | | | | | | | | | | |  | | | | | | | | | | |  | | | | | | | | | | | | |  | | | |
|  | | | | |  | | | Table S6 continued. | | | | | | | | | | | | |  | | | | | |  | | | | |  | | | | | | | | | | | | | | | | | | | | | | | | |
| Chemical | | | | | Atom | | | | | | | Id. # | | | | | ALogP\_AtomMRScore | | | | | | | | | | | | | Gasteiger\_Charges | | | | | VSA\_AtomicAreas | | | | | | | | | | VSA\_PartialCharge | | | | | | | | | | | Kappa\_3 | | | | |
| BDE-99 | | | | | C1  C1  C2  C3  C4  C5  Br6  Br7  O8  C9  C10  C11  C12  C13  C14  Br15  Br16  Br17  H1  H2  H3  H4  H5 | | | | | | | 0  0  1  2  3  4  5  6  7  8  9  10  11  12  13  14  15  16  17  1  2  3  4  5 | | | | | 3.4491  3.4491  3.7593  3.7593  3.4491  3.7593  8.2065  8.2065  1.3502  3.7593  3.4491  3.7593  3.7593  3.4491  3.7593  8.2065  8.2065  8.2065  0.8939  0.8939  0.8939  0.8939  0.8939 | | | | | | | | | | | | | -4.53e-002 -2.9e-002 9.63e-002 4.94e-002 -3.11e-002 1.88e-002 -5.08e-002 -4.79e-002 -0.308 9.74e-002 -1.47e-002 3.43e-002 3.3e-002 -2.99e-002 4.95e-002 -4.79e-002 -4.96e-002 -4.95e-002 6.35e-002 6.51e-002 6.47e-002 6.63e-002 6.54e-00 | | | | | 9.564 9.564 7.867 4.365 9.564 4.365 42.496 42.496 8.689 7.867 9.564 4.365 4.365 9.564 4.365 42.496 42.496 42.496 7.657 7.657 7.657 7.657 7.657 | | | | | | | | | | 8.689 0  0 0 0 42.496 217.804 21.828 54.022 0 0  0 0 0 | | | | | | | | | | | 3.52617 | | | | |
|  | | |  | | | | | Table S6continued. | | | | | | | | | | | | | | | | | | | | | |  | | | | |  | | | | | | | | | |  | | | | | | | | | | |  | | | | |
|  |  | | | |  | | | |  | | | | | | | | | | | | | | | | | | | | |  | | | | |  | | | | | | | | | |  | | | | | | | | | | |  | | | | |
| Chemical | | | | | | Atom | | | | | | Id. # | | | | ALogP\_AtomMRScore | | | | | | | | | | | | Gasteiger\_Charges | | | | | | | | | VSA\_AtomicAreas | | | | | | | | | | | VSA\_PartialCharge | | | | | | | | | | Kappa\_3 | | |
| PBDE-100 | | | | | | Br1  C1  C2  O3  C4  C5  Br6  C7  C8  Br9  C10  C11  C12  Br13  C14  C15  Br16  C17  H1  H2  H3  H4  H5 | | | | | | 0  0  1  2  3  4  5  6  7  8  9  10  11  12  13  14  15  16  17  1  2  3  4  5 | | | | 3.4491  3.4491  3.7593  3.7593  3.4491  3.7593  8.2065  8.2065  1.3502  3.7593  3.7593  3.4491  3.7593  3.4491  3.7593  8.2065  8.2065  8.2065  0.8939  0.8939  0.8939  0.8939  0.8939 | | | | | | | | | | | | -4.53e-002 -2.9e-002 9.63e-002 4.94e-002 -3.11e-002 1.88e-002 -5.08e-002 -4.79e-002 -0.3069 0.1105 5.06e-002 -3.1e-002 1.99e-002 -3.1e-002 5.06e-002 -4.79e-002 -5.08e-002 -4.79e-002 6.35e-002 6.51e-002 6.47e-002 6.47e-002 6.55e-002 | | | | | | | | | 9.564 9.564 7.867 4.365 9.564 4.365 42.496 42.496 8.689 7.867 4.365 9.564 4.365 9.564 4.365 42.496 42.496 42.496 7.657 7.657 7.657 7.657 7.657 | | | | | | | | | | | 8.689 0 0 0 0 84.992 175.308 13.097 54.886 7.867 0 0 0 0 | | | | | | | | | | 3.52617 | | |
|  |  | | | |  | | | |  | | | | | | | | | | | | | | |  | | | | | | | | | |  | | | | | | | | | | |  | | | | | | | | | | |  | | | | |
|  | | |  | | | | | Table S6continued. | | | | | | | | | | | | | | | | |  | | | | | | | | | | | | | | | | |  |
|  | | |  | | | | |  | | | | | | | | | | | |  | | | | |  | | | | | | | | | | | | | | | | |  |
| Chemical | | | | Atom | | | | | | | | Id. | | | | | | ALogP\_AtomMRScore | | | | | | | | | | | | Gasteiger\_Charges | | | | | | | VSA\_AtomicAreas | | | | | | | | | | VSA\_PartialCharge | | | | | | | | | | | Kappa\_3 | | |
| PBDE-153 | | | | C1  C1  C2  C3  C4  C5  Br6  Br7  Br8  O9  C10  C11  C12  C13  C14  C15  Br16  Br17  Br18  H1  H2  H3  H4 | | | | | | | | 0  1  2  3  4  5  6  7  8  9  10  11  12  13  14  15  16  17  18  1  2  3  4 | | | | | | 3.4491  3.7593  3.7593  3.4491  3.7593  3.7593  8.2065  8.2065  8.2065  1.3502  3.7593  3.4491  3.7593  3.7593  3.4491  3.7593  8.2065  8.2065  8.2065  0.8939  0.8939  0.8939  0.8939 | | | | | | | | | | | | -1.47e-002 9.74e-002 4.95e-002 -2.99e-002 3.3e-002 3.43e-002 -4.95e-002 -4.96e-002 -4.79e-002 -0.308 9.74e-002 -1.47e-002 3.43e-002 3.3e-002 -2.99e-002 4.95e-002 -4.79e-002 -4.96e-002 -4.95e-002 6.63e-002 6.47e-002 6.63e-002 6.55e-00 | | | | | | | 9.564 7.867 4.365 9.564 4.365 4.365 42.496 42.496 42.496 8.689 7.867 9.564 4.365 4.365 9.564 4.365 42.496 42.496 42.496 7.657 7.657 7.657 7.657 | | | | | | | | | | 8.689 0 0 0 0 0 293.232 26.194 46.364 0 0 0 0 0 | | | | | | | | | | | 3.55555 | | |
|  | | |  | | | | | Table S6continued. | | | | | | | | | | | | | | | | |  | | | | | | | | | | | | | | | | |  |
| Chemical | | | | | | | Atom | | | | | Id. # | | | | ALogP\_AtomMRScore | | | | | | | | | | | | Gasteiger\_Charges | | | | | | | | VSA\_AtomicAreas | | | | | | | | | | VSA\_PartialCharge | | | | | | | | | | | | | Kappa\_3 | | |
| PBDE-183 | | | | | | | C1  C1  C2  C3  C4  C5  Br6  Br7  Br8  O9  C10  C11  C12  C13  C14  C15  Br16  Br17  Br18  Br19  H1  H2  H3 | | | | | 0  1  2  3  4  5  6  7  8  9  10  11  12  13  14  15  16  17  18  19  1  2  3 | | | | 8.2065  3.7593  3.4491  3.7593  8.2065  3.7593  8.2065  3.7593  8.2065  3.7593  1.3502  3.7593  3.7593  8.2065  3.4491  3.7593  8.2065  3.7593  8.2065  3.4491  0.8939  0.8939  0.8939 | | | | | | | | | | | | -4.79e-002 5.06e-002 -2.99e-002 3.41e-002 -4.95e-002 4.86e-002 -4.83e-002 6.48e-002 -4.67e-002 0.1116 -0.3068 9.75e-002 4.95e-002 -4.79e-002 -2.99e-002 3.3e-002 -4.96e-002 3.43e-002 -4.95e-002 -1.47e-002 6.47e-002 6.47e-002 6.73e-002 | | | | | | | | 42.496 4.365 9.564 4.365 42.496 4.365 42.496 4.365 42.496 7.867 8.689 7.867 4.365 42.496 9.564 4.365 42.496 4.365 42.496 9.564 7.657 7.657 7.657 | | | | | | | | | | 8.689 0 0 0 0 0 326.164 21.828 39.571 7.867 0 0 0 0 | | | | | | | | | | | | | 3.4425 | | |
|  | | | | | | |  | | | | |  | | | |  | | | | | | | | | | | |  | | | | | | | |  | | | | | | | | | |  | | | | | | | | | | | | |  | | |
|  | | | | | | |  | | | | |  | | | |  | | | | | | | | | | | |  | | | | | | | |  | | | | | | | | | |  | | | | | | | | | | | | |  | | |
|  | | |  | | | | | Table S6continued. | | | | | | | | | | | | | | | | | | | | | | |  | | | | | | | | | | |  |
| Chemical | | | | | Atom | | | | | | | | Id. # | | | | | ALogP\_AtomMRScore | | | | | | | | | | | | | Gasteiger\_Charges | | | | | | | | | VSA\_AtomicAreas | | | | | | | | | | | | VSA\_PartialCharge | | | | | | | | Kappa\_3 | |
| PBDE-209 | | | | | C1  C1  C2  C3  C4  C5  Br6  Br7  Br8  Br9  Br10  O11  C12  C13  C14  C15  C16  C17  Br18  Br19  Br20  Br21  Br22 | | | | | | | | 0  1  2  3  4  5  6  7  8  9  10  11  12  13  14  15  16  17  18  19  20  21  22 | | | | | 3.7593  3.7593  3.7593  3.7593  3.7593  3.7593  8.2065  8.2065  8.2065  8.2065  8.2065  1.3502  3.7593  3.7593  3.7593  3.7593  3.7593  3.7593  8.2065  8.2065  8.2065  8.2065  8.2065 | | | | | | | | | | | | | 0.1128 6.48e-002 4.97e-002 4.83e-002 4.97e-002 6.48e-002 -4.66e-002 -4.82e-002 -4.83e-002 -4.82e-002 -4.66e-002 -0.3055 0.1128 6.48e-002 4.97e-002 4.83e-002 4.97e-002 6.48e-002 -4.66e-002 -4.82e-002 -4.83e-002 -4.82e-002 -4.55e-002 | | | | | | | | | 7.867 4.365 4.365 4.365 4.365 4.365 42.496 42.496 42.496 42.496 42.496 8.689 7.867 4.365 4.365 4.365 4.365 4.365 42.496 42.496 42.496 42.496 42.496 | | | | | | | | | | | | 8.689 0 0 0 0 0 424.96 26.194 17.462 15.734 0 0 0 0 | | | | | | | | 3.25443 | |
|  | | | | |  | | | | | | | |  | | | | |  | | | | | | | | | | | | |  | | | | | | | | |  | | | | | | | | | | | |  | | | | | | | |  | |
|  | | |  | | | | | Table S6continued. | | | | | | | | | | | | | | | | | | | | | | |  | | | | | | | | | | |  | | | | | | | | | | |
| Chemical | | | | | | Atom | | | | | | | Id. # | | | | | | ALogP\_AtomMRScore | | | | | | | | | | | | Gasteiger\_Charges | | | | | | | | | | VSA\_AtomicAreas | | | | | | | | | | | | VSA\_PartialCharge | | Kappa\_3 | | | | | |
| 3-OH-BDE-47 | | | | | | C1  C1  C2  C3  C4  C5  Br6  Br7  O8  C9  C10  C11  C12  C13  C14  Br15  Br16  H1  H2  H3  H5  H6  O24 | | | | | | | 0  1  2  3  4  5  6  7  8  9  10  11  12  13  14  15  16  1  2  3  5  6  24 | | | | | | 3.4491  3.4491  3.7593  3.7593  3.7593  3.7593  8.2065  8.2065  1.3502  3.7593  3.7593  3.4491  3.7593  3.4491  3.4491  8.2065  8.2065  -999  0.8939  0.8939  0.8939  0.8939  0.8939 | | | | | | | | | | | | -4.14e-002 -2.87e-002 0.1002 9.68e-002 0.209 6.62e-002 -4.66e-002 -4.37e-002 -0.308 9.63e-002 4.94e-002 -3.11e-002 1.87e-002 -4.53e-002 -2.9e-002 -5.08e-002 -4.8e-002 -1.2873 6.36e-002 6.51e-002 6.47e-002 6.35e-002 6.640e- | | | | | | | | | | 9.564 9.564 7.867 4.365 7.867 4.365 42.496 42.496 8.689 7.867 4.365 9.564 4.365 9.564 9.564 42.496 42.496 15.795 7.657 7.657 7.657 7.657 7.657 | | | | | | | | | | | | 24.485 0 0 0 0 42.496 175.308 8.731 54.886 7.867 0 7.867 0 0 | | 3.32179 | | | | | |
|  | | |  | | | | | Table S6continued. | | | | | | | | | | | | | | | | |  | | | | | | | | | | | | | | | | |  | | | | | | | | |
| Chemical | | | | | Atom | | | | | | | | | Id.# | | | | ALogP\_AtomMRScore | | | | | | | | | | | Gasteiger\_Charges | | | | | | | | | | VSA\_AtomicAreas | | | | | | | | | | | | VSA\_PartialCharge | | | | | | | | Kappa\_3 | |
| 5-OH-BDE-47 | | | | | C1  C1  C2  C3  C4  C5  Br6  Br7  O8  C9  C10  C11  C12  C13  C14  Br15  Br16  O18  H19  H2  H3  H4  H5  H6 | | | | | | | | | 0  1  2  3  4  5  6  7  8  9  10  11  12  13  14  15  16  18  19  2  3  4  5  6  6 | | | | 3.7593  3.4491  3.7593  3.7593  3.4491  3.7593  8.2065  8.2065  1.3502  3.7593  3.7593  3.4491  3.7593  3.4491  3.4491  8.2065  8.2065  -999  0.8939  0.8939  0.8939  0.8939  0.8939 | | | | | | | | | | | 0.1949 1.86e-002 0.1002 4.97e-002 -2.71e-002 6.61e-002 -4.66e-002 -4.8e-002 -0.308 9.63e-002 4.94e-002  -3.11e-002 1.87e-002 -4.53e-002 -2.9e-002 -5.08e-002 -4.8e-002 -1.2886 6.92e-002 6.48e-002 6.47e-002 6.35e-002 6.640e-002 | | | | | | | | | | 7.867 9.564 7.867 4.365 9.564 4.365 42.496 42.496 8.689 7.867 4.365 9.564 4.365 9.564 9.564 42.496 42.496 15.795 7.657 7.657 7.657 7.657 7.657 | | | | | | | | | | | | 24.485 0 0 0 0 42.496 165.744 22.661 50.52 7.867 7.867 0 0 0 | | | | | | | | 3.52617 | |
|  | | |  | | | | | Table S6 continued. | | | | | | | | | | | | | | | | |  | | | | | | | | | | | | | | | | |  | | | | | | | | |
| Chemical | | | | | | Atom | | | | | Id. # | | | | | ALogP\_AtomMRScore | | | | | | | | | | Gasteiger\_Charges | | | | | | | | | | | | VSA\_AtomicAreas | | | | | | | | | | | VSA\_PartialCharge | | | | | | | | Kappa\_3 | | | |
| 6-OH-BDE-47 | | | | | | C1  C1  C2  C3  C4  C5  Br6  Br7  O8  C9  C10  C11  C12  C13  C14  Br15  Br16  O18  H19  H2  H3  H4  H5  H6 | | | | | 01  2  3  4  5  6  7  8  9  10  11  12  13  14  15  16  17  18  2  3  4  5  6 | | | | | 3.4491  3.7593  3.7593  3.7593  3.4491  3.7593  8.2065  8.2065  1.3502  3.7593  3.7593  3.4491  3.7593  3.4491  3.4491  8.2065  8.2065  -999  0.8939  0.8939  0.8939  0.8939  0.8939 | | | | | | | | | | 2.5e-003 0.211 0.1435 5.34e-002 -3.08e-002 2.26e-002 -5.07e-002 -4.78e-002 -0.304 9.65e-002 4.94e-002 -3.11e-002 1.87e-002 -4.53e-002 -2.9e-002 -5.08e-002 -4.8e-002 -1.2869 6.76e-002 6.47e-002 6.47e-002 6.35e-002 6.630e-002 | | | | | | | | | | | | 9.564 7.867 7.867 4.365 9.564 4.365 42.496 42.496 8.689 7.867 4.365 9.564 4.365 9.564 9.564 42.496 42.496 15.795 7.657 7.657 7.657 7.657 7.657 | | | | | | | | | | | 24.485 0 0 0 0 84.992 123.248 22.661 50.52 7.867 0 7.867 0 0 | | | | | | | | 3.52617 | | | |
|  | |  | | | | | | | | |  | | | | |  | | | | | | |  | | | | | | | | | | | | | | | |  | | | | | | | | | | |  | | | |  | | | | | | |