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 | C1C1C2C3C4C5O6C7C8C9C10C11C12Br13Br14Br15H1H2H3H4H5H6H7 | 01234567891011121314151234567 | 8.20653.75933.44913.75938.20653.44913.44913.75931.35023.75933.44913.44913.75938.20653.44913.44910.89390.89390.89390.89390.89390.89390.8939 | -4.79e-0024.94e-002-3.11e-0021.88e-002-5.08e-002-4.53e-002-2.9e-0029.62e-002-0.30938.21e-002-3.02e-002-4.54e-0021.76e-002-5.09e-002-4.54e-002-3.02e-0026.47e-0026.35e-0026.51e-0026.5e-0026.35e-0026.35e-0026.61e-002 | 42.4964.3659.5644.36542.4969.5649.5647.8678.6897.8679.5649.5644.36542.4969.5649.5647.6577.6577.6577.6577.6577.6577.657 | 8.689000084.992109.44413.09769.33700000 |  3.49519 |

Table S6continued

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Chemical | Atom | Id. # | ALogP\_AtomMRScore | Gasteiger\_Charges | VSA\_AtomicAreas | VSA\_PartialCharge | Kappa\_3 |
| BDE-47 |   C1C1C2C3C4C5Br6Br7O8C9C10C11C12C13C14Br15Br16H1H2H3H4H5H6 |   012345678910111213141516123456 | 3.44913.44913.75933.75933.44913.75938.20658.20651.35023.75933.75933.44913.75933.44913.44918.20658.20650.89390.89390.89390.89390.89390.8939 | -4.53e-002-2.9e-0029.63e-0024.94e-002-3.11e-0021.88e-002-5.08e-002-4.79e-002-0.30819.63e-0024.94e-002-3.11e-0021.88e-002-4.53e-002-2.9e-002-5.08e-002-4.79e-0026.35e-0026.51e-0026.47e-0026.47e-0026.35e-0026.58000 | 9.5649.5647.8674.3659.5644.36542.49642.4968.6897.8674.3659.5644.3659.5649.56442.49642.4967.6577.6577.6577.6577.6577.657 | 8.689000084.992142.37617.46261.67900000 | 3.48444 |
|  |  |  |  |  |  |  |  |
|  |  | Table S6 continued. |  |  |  |
| Chemical | Atom  | Id. # | ALogP\_AtomMRScore | Gasteiger\_Charges | VSA\_AtomicAreas | VSA\_PartialCharge | Kappa\_3 |
| BDE-99 | C1C1C2C3C4C5Br6Br7O8C9C10C11C12C13C14Br15Br16Br17H1H2H3H4H5 | 00123456789101112131415161712345 |  3.44913.44913.75933.75933.44913.75938.20658.20651.35023.75933.44913.75933.75933.44913.75938.20658.20658.20650.89390.89390.89390.89390.8939 | -4.53e-002-2.9e-0029.63e-0024.94e-002-3.11e-0021.88e-002-5.08e-002-4.79e-002-0.3089.74e-002-1.47e-0023.43e-0023.3e-002-2.99e-0024.95e-002-4.79e-002-4.96e-002-4.95e-0026.35e-0026.51e-0026.47e-0026.63e-0026.54e-00 | 9.5649.5647.8674.3659.5644.36542.49642.4968.6897.8679.5644.3654.3659.5644.36542.49642.49642.4967.6577.6577.6577.6577.657 | 8.689000042.496217.80421.82854.02200000 | 3.52617 |
|  |  | Table S6continued.  |  |  |  |  |
|  |  |  |  |  |  |  |  |
| Chemical | Atom | Id. # | ALogP\_AtomMRScore | Gasteiger\_Charges | VSA\_AtomicAreas | VSA\_PartialCharge | Kappa\_3 |
| PBDE-100 | Br1C1C2O3C4C5Br6C7C8Br9C10C11C12Br13C14C15Br16C17H1H2H3H4H5 | 00123456789101112131415161712345 | 3.44913.44913.75933.75933.44913.75938.20658.20651.35023.75933.75933.44913.75933.44913.75938.20658.20658.20650.89390.89390.89390.89390.8939 | -4.53e-002-2.9e-0029.63e-0024.94e-002-3.11e-0021.88e-002-5.08e-002-4.79e-002-0.30690.11055.06e-002-3.1e-0021.99e-002-3.1e-0025.06e-002-4.79e-002-5.08e-002-4.79e-0026.35e-0026.51e-0026.47e-0026.47e-0026.55e-002 | 9.5649.5647.8674.3659.5644.36542.49642.4968.6897.8674.3659.5644.3659.5644.36542.49642.49642.4967.6577.6577.6577.6577.657 | 8.689000084.992175.30813.09754.8867.8670000 | 3.52617 |
|  |  |  |  |  |  |  |  |
|  |  | Table S6continued.  |  |  |
|  |  |  |  |  |  |
| Chemical | Atom | Id. | ALogP\_AtomMRScore | Gasteiger\_Charges | VSA\_AtomicAreas | VSA\_PartialCharge | Kappa\_3 |
| PBDE-153 | C1C1C2C3C4C5Br6Br7Br8O9C10C11C12C13C14C15Br16Br17Br18H1H2H3H4 | 01234567891011121314151617181234 | 3.44913.75933.75933.44913.75933.75938.20658.20658.20651.35023.75933.44913.75933.75933.44913.75938.20658.20658.20650.89390.89390.89390.8939 | -1.47e-0029.74e-0024.95e-002-2.99e-0023.3e-0023.43e-002-4.95e-002-4.96e-002-4.79e-002-0.3089.74e-002-1.47e-0023.43e-0023.3e-002-2.99e-0024.95e-002-4.79e-002-4.96e-002-4.95e-0026.63e-0026.47e-0026.63e-0026.55e-00 | 9.5647.8674.3659.5644.3654.36542.49642.49642.4968.6897.8679.5644.3654.3659.5644.36542.49642.49642.4967.6577.6577.6577.657 | 8.68900000293.23226.19446.36400000 | 3.55555 |
|  |  | Table S6continued.  |  |  |
| Chemical |  Atom | Id. # | ALogP\_AtomMRScore | Gasteiger\_Charges | VSA\_AtomicAreas | VSA\_PartialCharge | Kappa\_3 |
| PBDE-183 | C1C1C2C3C4C5Br6Br7Br8O9C10C11C12C13C14C15Br16Br17Br18Br19H1H2H3 | 012345678910111213141516171819123 | 8.20653.75933.44913.75938.20653.75938.20653.75938.20653.75931.35023.75933.75938.20653.44913.75938.20653.75938.20653.44910.89390.89390.8939 | -4.79e-0025.06e-002-2.99e-0023.41e-002-4.95e-0024.86e-002-4.83e-0026.48e-002-4.67e-0020.1116-0.30689.75e-0024.95e-002-4.79e-002-2.99e-0023.3e-002-4.96e-0023.43e-002-4.95e-002-1.47e-0026.47e-0026.47e-0026.73e-002 | 42.4964.3659.5644.36542.4964.36542.4964.36542.4967.8678.6897.8674.36542.4969.5644.36542.4964.36542.4969.5647.6577.6577.657 | 8.68900000326.16421.82839.5717.8670000 |  3.4425 |
|  |  |  |  |  |  |  |  |
|  |  |  |  |  |  |  |  |
|  |  | Table S6continued.  |  |  |
| Chemical | Atom | Id. # | ALogP\_AtomMRScore | Gasteiger\_Charges | VSA\_AtomicAreas | VSA\_PartialCharge | Kappa\_3 |
| PBDE-209 | C1C1C2C3C4C5Br6Br7Br8Br9Br10O11C12C13C14C15C16C17Br18Br19Br20Br21Br22 | 012345678910111213141516171819202122 | 3.75933.75933.75933.75933.75933.75938.20658.20658.20658.20658.20651.35023.75933.75933.75933.75933.75933.75938.20658.20658.20658.20658.2065 | 0.11286.48e-0024.97e-0024.83e-0024.97e-0026.48e-002-4.66e-002-4.82e-002-4.83e-002-4.82e-002-4.66e-002-0.30550.11286.48e-0024.97e-0024.83e-0024.97e-0026.48e-002-4.66e-002-4.82e-002-4.83e-002-4.82e-002-4.55e-002 | 7.8674.3654.3654.3654.3654.36542.49642.49642.49642.49642.4968.6897.8674.3654.3654.3654.3654.36542.49642.49642.49642.49642.496 | 8.68900000424.9626.19417.46215.7340000 | 3.25443 |
|  |  |  |  |  |  |  |  |
|  |  | Table S6continued.  |  |  |
| Chemical | Atom | Id. # | ALogP\_AtomMRScore | Gasteiger\_Charges | VSA\_AtomicAreas | VSA\_PartialCharge | Kappa\_3 |
| 3-OH-BDE-47 | C1C1C2C3C4C5Br6Br7O8C9C10C11C12C13C14Br15Br16H1H2H3H5H6O24 | 0123456789101112131415161235624 | 3.44913.44913.75933.75933.75933.75938.20658.20651.35023.75933.75933.44913.75933.44913.44918.20658.2065-9990.89390.89390.89390.89390.8939 | -4.14e-002-2.87e-0020.10029.68e-0020.2096.62e-002-4.66e-002-4.37e-002-0.3089.63e-0024.94e-002-3.11e-0021.87e-002-4.53e-002-2.9e-002-5.08e-002-4.8e-002-1.28736.36e-0026.51e-0026.47e-0026.35e-0026.640e- | 9.5649.5647.8674.3657.8674.36542.49642.4968.6897.8674.3659.5644.3659.5649.56442.49642.49615.7957.6577.6577.6577.6577.657 | 24.485000042.496175.3088.73154.8867.86707.86700 | 3.32179 |
|  |  | Table S6continued. |  |  |
| Chemical | Atom | Id.# | ALogP\_AtomMRScore | Gasteiger\_Charges | VSA\_AtomicAreas | VSA\_PartialCharge | Kappa\_3 |
| 5-OH-BDE-47 | C1C1C2C3C4C5Br6Br7O8C9C10C11C12C13C14Br15Br16O18H19H2H3H4H5H6 | 0123456789101112131415161819234566 |  3.75933.44913.75933.75933.44913.75938.20658.20651.35023.75933.75933.44913.75933.44913.44918.20658.2065-9990.89390.89390.89390.89390.8939 | 0.19491.86e-0020.10024.97e-002-2.71e-0026.61e-002-4.66e-002-4.8e-002-0.3089.63e-0024.94e-002-3.11e-0021.87e-002-4.53e-002-2.9e-002-5.08e-002-4.8e-002-1.28866.92e-0026.48e-0026.47e-0026.35e-0026.640e-002 | 7.8679.5647.8674.3659.5644.36542.49642.4968.6897.8674.3659.5644.3659.5649.56442.49642.49615.7957.6577.6577.6577.6577.657 | 24.485000042.496165.74422.66150.527.8677.867000 | 3.52617 |
|  |  | Table S6 continued. |  |  |
| Chemical | Atom | Id. # | ALogP\_AtomMRScore | Gasteiger\_Charges | VSA\_AtomicAreas | VSA\_PartialCharge | Kappa\_3 |
| 6-OH-BDE-47 | C1C1C2C3C4C5Br6Br7O8C9C10C11C12C13C14Br15Br16O18H19H2H3H4H5H6 | 012345678910111213141516171823456 | 3.44913.75933.75933.75933.44913.75938.20658.20651.35023.75933.75933.44913.75933.44913.44918.20658.2065-9990.89390.89390.89390.89390.8939 | 2.5e-0030.2110.14355.34e-002-3.08e-0022.26e-002-5.07e-002-4.78e-002-0.3049.65e-0024.94e-002-3.11e-0021.87e-002-4.53e-002-2.9e-002-5.08e-002-4.8e-002-1.28696.76e-0026.47e-0026.47e-0026.35e-0026.630e-002 | 9.5647.8677.8674.3659.5644.36542.49642.4968.6897.8674.3659.5644.3659.5649.56442.49642.49615.7957.6577.6577.6577.6577.657 | 24.485000084.992123.24822.66150.527.86707.86700 | 3.52617 |
|  |  |  |  |  |  |  |  |