**Additional supporting information**

**(for review)**

Decision-based QSAR model

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| S.No. | 2D Descriptors | Coefficient of Determination | MSE | Q2(LOO) | MSE(LOO) | MAE(LOO) | mean r2m (LOO) | delta rm2 (LOO) | Q2F1 | Q2F2 | MSE (test) | MAE (test) | r2m (test) | delta rm2 (test) |
| 1 | ['kappam2', 'GATSm6', 'GATSv2', 'ATSm4', 'radiust', 'CIC2', 'CIC3', 'IC4', 'bcutm16', 'bcutv13', 'CATS\_DD0', 'CATS\_DP4'] | 1 | 0 | 1.0 ± 0.0 | 0.0 ± 0.0 | 0.0 ± 0.0 | 1.0 ± 0.0 | 0.0 ± 0.0 | 0.579 | 0.578 | 1559557 | 668.242 | 0.578 | 0 |
| 2 | ['kappam2', 'GATSm6', 'GATSv2', 'ATSm4', 'radiust', 'CIC2', 'CIC3', 'IC4', 'bcutm16', 'bcutv13', 'CATS\_DD0', 'CATS\_AL5'] | 1 | 0 | 1.0 ± 0.0 | 0.0 ± 0.0 | 0.0 ± 0.0 | 1.0 ± 0.0 | 0.0 ± 0.0 | 0.077 | 0.075 | 3418649 | 1266.755 | 0.048 | 0.055 |
| 3 | ['kappam2', 'GATSm6', 'GATSv2', 'ATSm4', 'radiust', 'CIC2', 'CIC3', 'IC4', 'bcutm16', 'bcutv13', 'CATS\_DD0', 'CATS\_AL7'] | 1 | 0 | 1.0 ± 0.0 | 0.0 ± 0.0 | 0.0 ± 0.0 | 1.0 ± 0.0 | 0.0 ± 0.0 | 0.579 | 0.578 | 1558835 | 662.035 | 0.578 | 0 |
| 4 | ['kappam2', 'GATSm6', 'GATSv2', 'ATSm4', 'radiust', 'CIC2', 'CIC3', 'IC4', 'bcutm16', 'bcutv13', 'CATS\_DD0', 'CATS\_LL0'] | 1 | 0 | 1.0 ± 0.0 | 0.0 ± 0.0 | 0.0 ± 0.0 | 1.0 ± 0.0 | 0.0 ± 0.0 | 0.536 | 0.535 | 1719125 | 693.37 | 0.535 | 0 |
| 5 | ['kappam2', 'GATSm6', 'GATSv2', 'ATSm4', 'radiust', 'CIC2', 'CIC3', 'IC4', 'bcutm16', 'bcutv13', 'CATS\_DD0', 'CATS\_LL0'] | 1 | 0 | 1.0 ± 0.0 | 0.0 ± 0.0 | 0.0 ± 0.0 | 1.0 ± 0.0 | 0.0 ± 0.0 | 0.536 | 0.535 | 1719125 | 693.37 | 0.535 | 0 |

Regression-based QSAR model

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| S.No. | 2D Descriptors | Coefficient of Determination | MSE | Q2(LOO) | MSE(LOO) | MAE(LOO) | mean r2m (LOO) | delta rm2 (LOO) | Q2F1 | Q2F2 | MSE (test) | MAE (test) | r2m (test) | delta rm2 (test) |
| 1 | ['Chi6ch', 'S9', 'Smax34', 'GATSm8', 'PEOEVSA6', 'VSAEstate8', 'MATSm6', 'CIC2', 'IC4', 'bcutv9', 'CATS\_DP4', 'CATS\_DP5', 'CATS\_AL5', 'CATS\_AL7'] | 0.965 | 0.015 | 0.959 ± 0.0 | 0.013 ± 0.003 | 0.077 ± 0.009 | 0.953 ± 0.015 | 0.029 ± 0.015 | 0.292 | 0.171 | 0.434 | 0.578 | 0.171 | 0 |
| 2 | ['Chi6ch', 'S9', 'Smax34', 'GATSm8', 'GATSv6', 'PEOEVSA6', 'VSAEstate8', 'MATSm6', 'CIC2', 'bcutv9', 'CATS\_DP4', 'CATS\_DP5', 'CATS\_AL5', 'CATS\_AL7'] | 0.986 | 0.006 | 0.983 ± 0.0 | 0.005 ± 0.001 | 0.051 ± 0.007 | 0.985 ± 0.007 | 0.004 ± 0.011 | 0.159 | 0.016 | 0.516 | 0.557 | 0.016 | 0 |
| 3 | ['Chi6ch', 'S9', 'Smax34', 'GATSm8', 'GATSv6', 'PEOEVSA6', 'VSAEstate8', 'CIC2', 'IC4', 'bcutv9', 'CATS\_DP4', 'CATS\_DP5', 'CATS\_AL5', 'CATS\_AL7'] | 0.976 | 0.01 | 0.973 ± 0.0 | 0.009 ± 0.002 | 0.058 ± 0.006 | 0.97 ± 0.011 | 0.014 ± 0.015 | 0.015 | -0.153 | 0.604 | 0.659 | -0.153 | 0 |
| 4 | ['Chi6ch', 'S9', 'Smax34', 'GATSm8', 'GATSv6', 'PEOEVSA6', 'VSAEstate8', 'MATSm6', 'CIC2', 'IC4', 'bcutv9', 'CATS\_DP4', 'CATS\_DP5', 'CATS\_AL5'] | 0.994 | 0.003 | 0.993 ± 0.0 | 0.003 ± 0.0 | 0.036 ± 0.004 | 0.992 ± 0.005 | 0.003 ± 0.009 | -0.061 | -0.241 | 0.65 | 0.634 | -0.241 | 0 |