**Table S1. Test data set used in the study.** This data set contains 53 compounds and six molecular descriptors.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| CID | LogP | PSA | DC | AIRC | ArRC | BI |
| 3071 | 4.26 | 31.58 | 2 | 0 | 4 | 1.26 |
| 14692 | 3.64 | 56.30 | 2 | 0 | 4 | 1.17 |
| 45592 | 3.64 | 27.82 | 2 | 0 | 3 | 1.25 |
| 231168 | 4.16 | 15.79 | 1 | 0 | 3 | 1.37 |
| 273811 | 4.34 | 31.58 | 2 | 0 | 4 | 1.26 |
| 275194 | 3.64 | 27.82 | 2 | 0 | 3 | 1.48 |
| 347330 | 4.61 | 15.79 | 1 | 0 | 3 | 1.22 |
| 378604 | 4.41 | 20.72 | 1 | 0 | 4 | 1.13 |
| 378608 | 4.23 | 19.03 | 1 | 1 | 3 | 1.13 |
| 389556 | 4.26 | 31.58 | 2 | 0 | 4 | 1.18 |
| 412865 | 3.68 | 38.06 | 2 | 1 | 4 | 1.07 |
| 472137 | 3.79 | 27.82 | 2 | 0 | 3 | 1.18 |
| 472138 | 3.79 | 27.82 | 2 | 0 | 3 | 1.2 |
| 609935 | 2.99 | 41.81 | 2 | 0 | 3 | 1.67 |
| 659062 | 3.74 | 19.03 | 1 | 0 | 3 | 1.38 |
| 750123 | 2.67 | 19.03 | 1 | 1 | 2 | 1.46 |
| 849416 | 3.77 | 27.82 | 2 | 0 | 3 | 1.37 |
| 1988062 | 4.16 | 27.82 | 2 | 0 | 3 | 1.2 |
| 2037245 | 4.12 | 27.82 | 2 | 0 | 3 | 1.06 |
| 2063772 | 2.43 | 40.71 | 2 | 0 | 3 | 1.25 |
| 2163781 | 3.74 | 43.61 | 3 | 0 | 4 | 1.17 |
| 2907031 | 4.6 | 44.47 | 2 | 0 | 5 | 1.16 |
| 2940682 | 4.47 | 44.47 | 2 | 0 | 5 | 1.16 |
| 5221957 | 5.15 | 38.06 | 2 | 1 | 4 | 0.82 |
| 5889045 | 4.71 | 31.58 | 2 | 0 | 4 | 1.11 |
| 6035091 | 3.58 | 41.81 | 2 | 0 | 3 | 1.48 |
| 6618861 | 4.17 | 19.03 | 1 | 1 | 3 | 1.25 |
| 6917760 | 5.35 | 19.03 | 1 | 1 | 3 | 0.97 |
| 9820229 | 4.57 | 22.27 | 1 | 2 | 3 | 0.99 |
| 9948843 | 4.92 | 19.03 | 1 | 1 | 3 | 1.07 |
| 10086288 | 4.46 | 19.03 | 1 | 1 | 3 | 1.13 |
| 10089397 | 4.91 | 19.03 | 1 | 1 | 3 | 1.05 |
| 10900930 | 4.03 | 31.58 | 2 | 0 | 4 | 1.22 |
| 15547884 | 4.23 | 27.82 | 2 | 0 | 3 | 1.12 |
| 15619884 | 4.09 | 34.82 | 2 | 1 | 4 | 1.2 |
| 23370142 | 4.64 | 19.03 | 1 | 1 | 3 | 1.07 |
| 23370152 | 5.37 | 19.03 | 1 | 1 | 3 | 0.99 |
| 44230732 | 3.77 | 27.82 | 2 | 1 | 3 | 1.21 |
| 44230875 | 4.21 | 27.82 | 2 | 1 | 3 | 1.38 |
| 44231009 | 3.77 | 27.82 | 2 | 1 | 3 | 1.21 |
| 44303983 | 3.04 | 40.71 | 2 | 1 | 3 | 1.07 |
| 44405876 | 2.97 | 19.03 | 1 | 2 | 2 | 1.41 |
| 44589201 | 3.77 | 27.82 | 2 | 1 | 3 | 1.25 |
| 44589528 | 3.78 | 27.82 | 2 | 0 | 3 | 1.52 |
| 45267648 | 5.43 | 20.72 | 1 | 0 | 4 | 1.3 |
| 72164839 | 3.97 | 31.06 | 2 | 1 | 3 | 1.02 |
| 102500054 | 5.22 | 31.58 | 2 | 0 | 4 | 1.09 |
| 102500056 | 4.85 | 31.59 | 2 | 0 | 4 | 1.09 |
| 118709595 | 4.25 | 20.72 | 1 | 0 | 4 | 1.19 |
| 118732558 | 3.82 | 64.17 | 3 | 0 | 4 | 1.49 |
| 118732559 | 3.82 | 64.17 | 3 | 0 | 4 | 1.49 |
| 122187556 | 3.73 | 23.96 | 1 | 1 | 3 | 1.13 |
| 136244603 | 5.69 | 28.15 | 1 | 1 | 3 | 1.35 |

logP: Octanol-water partition coefficient

PSA: Polar surface area

DC: Donor count

AlRC: Aliphatic ring count

ArRC: Aromatic ring count

BI: Balaban index