**Table SM1.** The predicted/calculated and observed antioxidant activity values of CDs from model 3 and their descriptor and hat values.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Compound No** | **Observed**  **Log (AATEAC) (mM)** | **Predicted/Calculated**  **Log (AATEAC)**  **(mM) from model 3** | **Descriptors** | | **Hat values**  **(*h*\*=0.300)** |
| **IC2** | **CATS2D\_07\_DL** |
| Trolox | 0.0000 | 0.0221 | 3.815 | 3 | 0.0646 |
| 1 | 0.3554 | 0.4137 | 4.098 | 3 | 0.0794 |
| 2 | -0.7782 | -0.4992 | 4.265 | 0 | 0.1188 |
| 3 | 0.2871 | 0.0324 | 4.098 | 2 | 0.0546 |
| 4 | -0.3598 | -0.4992 | 4.265 | 0 | 0.1188 |
| 5\* | 0.5246 | 0.6824 | 3.741 | 5 | 0.1938 |
| 6 | -0.7869 | -0.6819 | 4.133 | 0 | 0.0834 |
| 7 | 0.2617 | 0.4137 | 4.098 | 3 | 0.0794 |
| 8\* | 0.3772 | 0.4137 | 4.098 | 3 | 0.0794 |
| 9 | 0.4249 | 0.7377 | 3.781 | 5 | 0.1889 |
| 10 | 0.3250 | 0.4137 | 4.098 | 3 | 0.0794 |
| 11 | -0.4859 | -0.4992 | 4.265 | 0 | 0.1188 |
| 12\* | 0.3132 | 0.5258 | 4.179 | 3 | 0.0969 |
| 13 | 0.5571 | 0.3362 | 4.042 | 3 | 0.0708 |
| 14 | 0.3579 | -0.1176 | 3.714 | 3 | 0.0767 |
| 15 | -0.7782 | -0.7923 | 3.502 | 2 | 0.1073 |
| 16 | 0.3032 | 0.3210 | 4.031 | 3 | 0.0694 |
| 17\* | -1.3310 | -1.1495 | 3.795 | 0 | 0.0640 |
| 18 | 0.0852 | -0.0803 | 3.741 | 3 | 0.0725 |
| 19 | -0.9720 | -1.2505 | 3.722 | 0 | 0.0733 |
| 20 | -1.7782 | -1.4000 | 3.614 | 0 | 0.0958 |
| 21\* | 0.4683 | 0.6824 | 3.741 | 5 | 0.1938 |
| 22 | -1.5740 | -1.4871 | 3.551 | 0 | 0.1137 |
| 23 | 0.4351 | 0.7377 | 3.781 | 5 | 0.1889 |
| 24\* | 0.0852 | -0.4970 | 3.991 | 1 | 0.0397 |
| 25 | 0.3338 | 0.1729 | 3.924 | 3 | 0.0618 |
| 26 | -0.6642 | -1.0651 | 3.856 | 0 | 0.0600 |
| 27 | -0.4859 | -0.6763 | 4.137 | 0 | 0.0843 |
| 28 | -0.7959 | -0.6556 | 4.152 | 0 | 0.0876 |
| 29 | 0.3509 | 0.1882 | 3.935 | 3 | 0.0621 |
| 30 | -0.8539 | -0.6473 | 4.158 | 0 | 0.0889 |
| 31 | -1.1549 | -0.8783 | 3.991 | 0 | 0.0628 |
| 32 | -1.0000 | -0.9863 | 3.913 | 0 | 0.0592 |
| 33\* | -0.8539 | -0.7331 | 4.096 | 0 | 0.0763 |
| 34 | -2.0000 | -2.0019 | 3.179 | 0 | 0.2922 |
| 35 | -2.0000 | -1.8441 | 3.293 | 0 | 0.2243 |
| 36 | -1.0000 | -1.1177 | 3.818 | 0 | 0.0621 |
| 37\* | -1.0969 | -0.9710 | 3.924 | 0 | 0.0594 |

\*Test set