**Table SM2.** The predicted antioxidant activity values of newly designed CDs from model 3 and their descriptor and hat values.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Compound No** | **Predicted**  **Log (AATEAC)**  **(mM) from model 3** | **Descriptors** | | **Hat values**  **(*h*\*=0.300)** |
| **IC2** | **CATS2D\_07\_DL** |
| E-32**≠** | 0.8365 | 4.128 | 4 | 0.1341 |
| E-33 | 1.3299 | 4.209 | 5 | 0.2267 |
| E-34 | **0.4552\*** | 4.128 | 3 | 0.0852 |
| E-35 | **0.7549** | 4.069 | 4 | 0.1234 |
| E-36 | **0.5756** | 4.215 | 3 | 0.1066 |
| E-37 | 0.8711 | 4.153 | 4 | 0.1395 |
| E-38 | **0.5756** | 4.215 | 3 | 0.1066 |
| E-39 | **0.2814** | 4.278 | 2 | 0.1013 |
| E-40 | 0.7983 | 4.376 | 3 | 0.1640 |
| E-41 | **0.1859** | 4.209 | 2 | 0.0799 |
| E-42 | 0.9486 | 4.209 | 4 | 0.1538 |
| E-43 | 1.2331 | 4.139 | 5 | 0.2093 |
| E-44 | 1.0192 | 4.260 | 4 | 0.1692 |
| E-45 | **0.1085** | 4.153 | 2 | 0.0657 |
| E-46 | **0.1818** | 4.206 | 2 | 0.0791 |
| E-47 | 0.8697 | 4.152 | 4 | 0.1393 |
| E-48 | **0.4137** | 4.098 | 3 | 0.0794 |
| E-56 | 0.9569 | 4.215 | 4 | 0.1555 |
| E-57 | **0.6337** | 4.257 | 3 | 0.1193 |
| E-58 | 0.8365 | 4.128 | 4 | 0.1341 |
| E-59 | **0.5548** | 4.200 | 3 | 0.1024 |
| E-60 | 0.7983 | 4.376 | 3 | 0.1640 |
| E-62 | **-0.6063** | 3.912 | 1 | 0.0360 |
| E-63 | 0.8551 | 4.417 | 3 | 0.1823 |
| E-64 | **0.1043** | 4.150 | 2 | 0.0651 |
| E-65 | **-0.3097** | 4.402 | 0 | 0.1721 |
| E-66 | **-0.1885** | 4.214 | 1 | 0.0803 |
| E-67 | **-0.1434** | 3.971 | 2 | 0.0391 |
| E-68 | **-0.3982** | 4.338 | 0 | 0.1451 |
| E-69 | **-0.2881** | 4.142 | 1 | 0.0623 |
| E-70 | **-0.2513** | 3.893 | 2 | 0.0368 |

≠ Compound numbers are the same as indicated in Table 5,

\*interpolated AA of CDs from model 3.