**Table S1** The residues of the examined molecules and their predicted and observed

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | pIC50 obs | pIC50 calculate | | | | | | | |
| CoMFA | Residus | CoMSIA  SEA | Residus | CoMSIA  SEH | Residus | CoMSIA  SEHDA | Residus |
| 1 | 5.6576 | 5.7012 | -0.0436 | 5.7123 | -0.0547 | 5.7719 | -0.1143 | 5.779 | -0.1214 |
| 2 | 6.0315 | 5.9947 | 0.0368 | 6.0511 | -0.0196 | 6.0993 | -0.0678 | 6.1026 | -0.0711 |
| 4 | 5.8416 | 5.8719 | -0.0303 | 5.8716 | -0.03 | 5.9934 | -0.1518 | 5.9875 | -0.1459 |
| 6 | 5.9245 | 5.946 | -0.0215 | 5.9425 | -0.018 | 5.8189 | 0.1056 | 5.822 | 0.1025 |
| 7 | 5.7520 | 5.7651 | -0.0131 | 5.7131 | 0.0389 | 5.6677 | 0.0843 | 5.6566 | 0.0954 |
| 8 | 6.2676 | 6.4775 | -0.2099 | 6.5126 | -0.245 | 6.4488 | -0.1812 | 6.448 | -0.1804 |
| 9 | 6.6383 | 6.5336 | 0.1047 | 6.5605 | 0.0778 | 6.4936 | 0.1447 | 6.4978 | 0.1405 |
| 10 | 6.4559 | 6.3539 | 0.102 | 6.3324 | 0.1235 | 6.3424 | 0.1135 | 6.3323 | 0.1236 |
| 11 | 5.9172 | 5.9483 | -0.0311 | 5.9199 | -0.0027 | 5.9464 | -0.0292 | 5.9799 | -0.0627 |
| 12 | 5.5952 | 5.5591 | 0.0361 | 5.5316 | 0.0636 | 5.591 | 0.0042 | 5.5792 | 0.016 |
| 13 | 5.5467 | 5.6131 | -0.0664 | 5.5789 | -0.0322 | 5.6354 | -0.0887 | 5.6285 | -0.0818 |
| 14 | 5.4522 | 5.2199 | 0.2323 | 5.2492 | 0.203 | 5.3517 | 0.1005 | 5.3641 | 0.0881 |
| 15 | 5.8508 | 5.6461 | 0.2047 | 5.6267 | 0.2241 | 5.6897 | 0.1611 | 5.6799 | 0.1709 |
| 16 | 5.6737 | 5.7035 | -0.0298 | 5.6782 | -0.0045 | 5.7374 | -0.0637 | 5.7325 | -0.0588 |
| 17 | 5.3536 | 5.3496 | 0.004 | 5.4181 | -0.0645 | 5.3709 | -0.0173 | 5.3697 | -0.0161 |
| 18 | 5.3188 | 5.4053 | -0.0865 | 5.4657 | -0.1469 | 5.4158 | -0.097 | 5.4195 | -0.1007 |
| 19 | 5.6737 | 5.7567 | -0.083 | 5.7163 | -0.0426 | 5.707 | -0.0333 | 5.6984 | -0.0247 |
| 20 | 5.9666 | 5.8111 | 0.1555 | 5.7657 | 0.2009 | 5.7528 | 0.2138 | 5.7492 | 0.2174 |
| 21 | 5.7799 | 5.8087 | -0.0288 | 5.7581 | 0.0218 | 5.793 | -0.0131 | 5.8095 | -0.0296 |
| 23 | 5.2262 | 5.2615 | -0.0353 | 5.2299 | -0.0037 | 5.1016 | 0.1246 | 5.1419 | 0.0843 |
| 24 | 5.1656 | 5.2866 | -0.121 | 5.3307 | -0.1651 | 5.2894 | -0.1238 | 5.2706 | -0.105 |
| 26 | 5.0706 | 5.1641 | -0.0935 | 5.1534 | -0.0828 | 5.185 | -0.1144 | 5.1572 | -0.0866 |
| 27 | 5.3635 | 5.2965 | 0.067 | 5.3265 | 0.037 | 5.2867 | 0.0768 | 5.2828 | 0.0807 |
| 28 | 5.2993 | 5.3488 | -0.0495 | 5.3775 | -0.0782 | 5.3329 | -0.0336 | 5.3339 | -0.0346 |
| 22\* | 5.857 | 5.8626 | -0.0056 | 5.8052 | 0.0518 | 5.8376 | 0.0194 | 5.8589 | -0.0019 |
| 25\* | 5.2993 | 5.3415 | -0.0422 | 5.3798 | -0.0805 | 5.3353 | -0.036 | 5.3214 | -0.0221 |
| 3\* | 6.3768 | 6.0514 | 0.3254 | 6.1029 | 0.2739 | 6.1468 | 0.23 | 6.1551 | 0.2217 |
| 29\* | 5.3197 | 4.8421 | 0.4776 | 4.9813 | 0.3384 | 5.1207 | 0.199 | 5.1580 | 0.1617 |
| 5\* | 5.8665 | 5.8877 | -0.0212 | 5.8918 | -0.0253 | 5.7727 | 0.0938 | 5.7708 | 0.0957 |