**Table S1.** 2D structures of chemical compounds and their biological activities of pKi order.

|  |  |  |
| --- | --- | --- |
| **1 pKi=6.703** | **2 pKi=6.701** | **3 pKi=5.821** |
| **4 pKi=7.745** | **5 pKi=5.903** | **6 pKi=****8.097** |
| **7 pKi=8.523** | **8 pKi=8.523** | **9 pKi=8.301** |
| **10 pKi=5.936** | **11 pKi=7.377** | **12 pKi=7.678** |
| **13 pKi=6.928** | **14 pKi=6.116** | **15 pKi=8.398** |
| **16 pKi=8.097** | **17 pKi=8.301** | **18 pKi=8.699** |
| **19 pKi=9.00** | **20 pKi=8.523** | **21 pKi=8.155** |
| **22 pKi=7.538** | **23 pKi=7.222** | **24 pKi=7.032** |
| **25 pKi=7.013** | **26 pKi=6.444** | **27 pKi=8.523** |
| **28 pKi=7.620** | **29 pKi=8.699** | **30 pKi=8.699** |

**Table S3.** The selected descriptors of studied compounds with inhibitory activities of pKi order

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **N°** | **% H** | **% C** | **% N** | **D** | **T E** | **VDW E** | **pKi** |
| 1 | 3.930 | 10.920 | 9.360 | 1.490 | 58.678 | 19.795 | 6.703 |
| 2\* | 5.800 | 14.650 | 8.370 | 1.310 | 35.378 | 18.322 | 6.701 |
| 3 | 6.100 | 14.130 | 8.070 | 1.290 | 36.789 | 19.478 | 5.821 |
| 4 | 6.100 | 14.130 | 8.070 | 1.290 | 34.719 | 18.945 | 7.745 |
| 5 | 6.100 | 14.130 | 8.070 | 1.290 | 34.680 | 18.964 | 5.903 |
| 6 | 4.700 | 12.440 | 7.100 | 1.400 | 39.322 | 18.992 | 8.097 |
| 7 | 4.300 | 11.960 | 6.830 | 1.440 | 39.315 | 18.886 | 8.523 |
| 8 | 4.640 | 12.880 | 7.360 | 1.430 | 35.361 | 18.733 | 8.523 |
| 9 | 3.940 | 11.520 | 6.580 | 1.480 | 40.323 | 18.962 | 8.301 |
| 10\* | 4.080 | 14.920 | 6.820 | 1.500 | 44.897 | 19.276 | 5.936 |
| 11\* | 4.640 | 12.880 | 7.360 | 1.430 | 35.363 | 18.728 | 7.377 |
| 12 | 4.640 | 12.880 | 7.360 | 1.430 | 35.991 | 18.930 | 7.678 |
| 13\* | 4.080 | 14.920 | 6.820 | 1.500 | 41.241 | 19.404 | 6.928 |
| 14 | 4.470 | 15.510 | 7.090 | 1.450 | 44.863 | 19.457 | 6.116 |
| 15 | 4.160 | 11.560 | 9.910 | 1.460 | 35.610 | 20.071 | 8.398 |
| 16 | 4.080 | 14.920 | 6.820 | 1.500 | 45.988 | 19.668 | 8.097 |
| 17 | 3.860 | 17.860 | 6.800 | 1.560 | 44.147 | 20.191 | 8.301 |
| 18 | 3.810 | 11.150 | 9.550 | 1.500 | 39.296 | 20.541 | 8.699 |
| 19\* | 5.720 | 12.720 | 7.260 | 1.400 | 40.735 | 19.063 | 9.000 |
| 20 | 3.720 | 14.370 | 6.560 | 1.540 | 40.651 | 18.898 | 8.523 |
| 21 | 4.240 | 8.410 | 12.810 | 1.430 | 38.144 | 22.613 | 8.155 |
| 22 | 3.850 | 8.450 | 12.860 | 1.460 | 39.408 | 22.598 | 7.538 |
| 23 | 4.450 | 11.240 | 9.630 | 1.430 | 35.626 | 20.613 | 7.222 |
| 24\* | 6.080 | 11.010 | 8.390 | 1.260 | 37.612 | 19.037 | 7.032 |
| 25 | 3.630 | 14.860 | 10.180 | 1.550 | 45.449 | 22.519 | 7.013 |
| 26 | 3.930 | 10.930 | 12.490 | 1.490 | 37.856 | 19.281 | 6.444 |
| 27 | 5.010 | 11.150 | 15.920 | 1.510 | 50.346 | 20.051 | 8.523 |
| 28 | 4.750 | 11.470 | 16.380 | 1.550 | 54.607 | 16.254 | 7.620 |
| 29 | 4.600 | 11.110 | 19.030 | 1.560 | 50.711 | 23.759 | 8.699 |
| 30 | 4.600 | 11.110 | 19.030 | 1.560 | 50.846 | 22.774 | 8.699 |

\* indicates the test set molecules

**Table S4.** The statistical results for 100 randomizations

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **Model** | ***R*** | ***R^2*** | ***Q^2*** | **Model** | ***R*** | ***R^2*** | ***Q^2*** |
| ***Original*** | ***0.864*** | ***0.746*** | ***0.529*** | Random N°51 | 0.678 | 0.460 | -0.035 |
| Random N°1 | 0.480 | 0.231 | -0.538 | Random N°52 | 0.443 | 0.196 | -0.454 |
| Random N°2 | 0.509 | 0.259 | -0.525 | Random N°53 | 0.373 | 0.139 | -1.193 |
| Random N°3 | 0.312 | 0.097 | -1.937 | Random N°54 | 0.628 | 0.395 | -0.172 |
| Random N°4 | 0.444 | 0.197 | -1.806 | Random N°55 | 0.380 | 0.144 | -0.836 |
| Random N°5 | 0.551 | 0.304 | -0.706 | Random N°56 | 0.384 | 0.148 | -0.877 |
| Random N°6 | 0.396 | 0.157 | -1.030 | Random N°57 | 0.489 | 0.239 | -0.676 |
| Random N°7 | 0.635 | 0.403 | -0.147 | Random N°58 | 0.621 | 0.385 | -0.195 |
| Random N°8 | 0.487 | 0.237 | -1.430 | Random N°59 | 0.603 | 0.364 | -0.365 |
| Random N°9 | 0.239 | 0.057 | -0.983 | Random N°60 | 0.433 | 0.188 | -1.198 |
| Random N°10 | 0.509 | 0.259 | -0.329 | Random N°61 | 0.633 | 0.401 | -0.534 |
| Random N°11 | 0.625 | 0.391 | -0.393 | Random N°62 | 0.423 | 0.179 | -0.626 |
| Random N°12 | 0.630 | 0.397 | -0.325 | Random N°63 | 0.575 | 0.330 | -0.297 |
| Random N°13 | 0.399 | 0.160 | -0.610 | Random N°64 | 0.341 | 0.117 | -1.395 |
| Random N°14 | 0.531 | 0.282 | -0.433 | Random N°65 | 0.533 | 0.284 | -1.631 |
| Random N°15 | 0.525 | 0.275 | -0.718 | Random N°66 | 0.537 | 0.288 | -0.405 |
| Random N°16 | 0.457 | 0.209 | -1.052 | Random N°67 | 0.300 | 0.090 | -1.331 |
| Random N°17 | 0.461 | 0.212 | -0.572 | Random N°68 | 0.301 | 0.091 | -1.246 |
| Random N°18 | 0.402 | 0.162 | -0.636 | Random N°69 | 0.559 | 0.312 | -0.433 |
| Random N°19 | 0.498 | 0.248 | -0.575 | Random N°70 | 0.481 | 0.231 | -0.631 |
| Random N°20 | 0.359 | 0.129 | -0.689 | Random N°71 | 0.519 | 0.269 | -0.555 |
| Random N°21 | 0.360 | 0.129 | -1.309 | Random N°72 | 0.431 | 0.185 | -0.476 |
| Random N°22 | 0.596 | 0.356 | -0.254 | Random N°73 | 0.587 | 0.345 | -0.247 |
| Random N°23 | 0.388 | 0.151 | -0.805 | Random N°74 | 0.661 | 0.436 | -0.024 |
| Random N°24 | 0.553 | 0.306 | -0.280 | Random N°75 | 0.326 | 0.106 | -0.920 |
| Random N°25 | 0.467 | 0.218 | -0.551 | Random N°76 | 0.490 | 0.240 | -0.382 |
| Random N°26 | 0.407 | 0.166 | -0.496 | Random N°77 | 0.473 | 0.224 | -0.471 |
| Random N°27 | 0.598 | 0.357 | -0.196 | Random N°78 | 0.655 | 0.430 | -0.000 |
| Random N°28 | 0.411 | 0.169 | -0.526 | Random N°79 | 0.388 | 0.151 | -0.682 |
| Random N°29 | 0.500 | 0.250 | -0.549 | Random N°80 | 0.359 | 0.129 | -1.036 |
| Random N°30 | 0.602 | 0.362 | -0.318 | Random N°81 | 0.633 | 0.401 | -0.616 |
| Random N°31 | 0.540 | 0.291 | -0.907 | Random N°82 | 0.545 | 0.297 | -0.527 |
| Random N°32 | 0.476 | 0.227 | -1.029 | Random N°83 | 0.381 | 0.145 | -0.621 |
| Random N°33 | 0.535 | 0.286 | -0.267 | Random N°84 | 0.614 | 0.377 | -0.388 |
| Random N°34 | 0.294 | 0.086 | -0.877 | Random N°85 | 0.734 | 0.539 | 0.001 |
| Random N°35 | 0.381 | 0.145 | -0.634 | Random N°86 | 0.329 | 0.108 | -0.672 |
| Random N°36 | 0.452 | 0.205 | -0.551 | Random N°87 | 0.655 | 0.429 | -0.300 |
| Random N°37 | 0.471 | 0.222 | -0.889 | Random N°88 | 0.374 | 0.140 | -0.670 |
| Random N°38 | 0.620 | 0.385 | -0.337 | Random N°89 | 0.279 | 0.078 | -0.518 |
| Random N°39 | 0.523 | 0.273 | -0.278 | Random N°90 | 0.726 | 0.528 | 0.055 |
| Random N°40 | 0.629 | 0.395 | 0.012 | Random N°91 | 0.341 | 0.116 | -1.155 |
| Random N°41 | 0.239 | 0.057 | -0.960 | Random N°92 | 0.459 | 0.211 | -0.353 |
| Random N°42 | 0.482 | 0.233 | -0.791 | Random N°93 | 0.435 | 0.189 | -0.666 |
| Random N°43 | 0.449 | 0.202 | -0.517 | Random N°94 | 0.339 | 0.115 | -2.102 |
| Random N°44 | 0.400 | 0.160 | -1.292 | Random N°95 | 0.655 | 0.429 | -0.417 |
| Random N°45 | 0.428 | 0.184 | -0.829 | Random N°96 | 0.288 | 0.083 | -1.104 |
| Random N°46 | 0.398 | 0.159 | -0.538 | Random N°97 | 0.264 | 0.070 | -0.982 |
| Random N°47 | 0.692 | 0.479 | -0.063 | Random N°98 | 0.396 | 0.156 | -1.175 |
| Random N°48 | 0.385 | 0.148 | -0.990 | Random N°99 | 0.464 | 0.216 | -0.511 |
| Random N°49 | 0.408 | 0.166 | -0.569 | Random N°100 | 0.494 | 0.244 | -0.755 |
| Random N°50 | 0.699 | 0.489 | -0.141 |  |  |  |  |