**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  |  |  |  |  |