**Supplementary Sable S1:** Volume and Area of top ten pocket of human aurora kinase B (AURKB) protein

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **PocID** | **N\_mth** | **Area (SA) Å2** | **Area\_ms** | **Volume (SA) Å3** | **Vol\_ms** | **Lenth** | **cnr** |
| 1 | 3 | 1422.221 | 1951.636 | 2269.76 | 4609.11 | 1082.368 | 465 |
| 2 | 1 | 255.877 | 452.748 | 191.801 | 678.497 | 239.321 | 117 |
| 3 | 1 | 107.138 | 184.001 | 85.996 | 289.924 | 108.508 | 48 |
| 4 | 1 | 51.835 | 106.97 | 29.832 | 138.573 | 56.285 | 29 |
| 5 | 1 | 47.659 | 82.85 | 26.58 | 117.318 | 47.563 | 21 |
| 6 | 1 | 50.204 | 167.681 | 22.24 | 154.406 | 64.056 | 37 |
| 7 | 1 | 35.989 | 68.482 | 16.191 | 85.501 | 31.81 | 19 |
| 8 | 1 | 7.036 | 9.561 | 7.626 | 20.523 | 6.216 | 1 |
| 9 | 1 | 19.481 | 70.188 | 5.533 | 65.629 | 28.924 | 15 |
| 10 | 1 | 13.633 | 43.554 | 4.082 | 43.073 | 16.778 | 9 |

**Supplementary Table S2:** Autodock vina predicts the binding strengths of the top four compounds and the control (CID: 24139). It also gives the compound ID, IUPAC chemical name, and 2D structure.

|  |  |  |  |
| --- | --- | --- | --- |
| **Compound ID** | **Chemical Name (IUPAC)** | **2D structure** | **Binding affinity (kcal/mol)** |
| **CID:**16273992 | 2-(4-oxo-[1]benzofuro[3,2-d]pyrimidin-3-yl)-N-[2-(1,2,4-triazol-1-yl)-5-(trifluoromethyl)phenyl]acetamide |  | -10.6 |
| **CID:**16273736 | [2-(4-chloro-2- methoxy-5-methylanilino)- 2-oxoethyl] 9,10,10-trioxothioxanthene-3-carboxylate |  | -10.5 |
| **CID:**8895340 | methyl 3-[2-(4-nitro-1,3-dioxoisoindol-2-yl)acetyl]oxybenzoate |  | -9.9 |
| **CID:**16272857 | 2-chloro-N-(2,4-dimethylphenyl)-5 ,5-dioxo-8,9,10,11-tetrahydro-7H-azepino[2,1-c][1,2,4]benzothiadiazine-3-carboxamide |  | -9.9 |
| **CID:**  16273739 | [2-oxo- 2-(2-oxopyrrolidin-1-yl)ethyl] 1-oxo-3-phenyl-3,4-dihydroisochromene-6-carboxylate |  | -9.8 |
| **CID:**  5494449  **(Control)** | Tozasertib |  | -9.4 |