|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **IDNUMBER** | **docking with 6Y9S\_A**  | **prime MMGBSA****dG\_Bind** | **inhibition(20μg/mL)** | **IC50(μM)** |
| **SP score** | **XP score** | **rate(%)** | **SD(%)** | **IC50(μM)** | **SD** |
| **AG-205/36495010** | **-6.89**  | **-9.10**  | **-53.08**  | **2.13** | **0.46** |  |  |
| **AG-690/13155009** | **-8.93**  | **-7.64**  | **-58.90**  | **4.08** | **4.73** |  |  |
| **AK-777/09836064** | **-7.93**  | **-8.70**  | **-51.51**  | **60.39** | **0.9** | **15.5** | **1.57** |
| **AK-968/37185006** | **-8.38**  | **-7.92**  | **-61.22**  | **88.71** | **1.54** | **17.42** | **2.85** |
| **AN-698/41607072** | **-7.64**  | **-8.38**  | **-67.92**  | **50.17** | **5.61** | **6.74** | **1.05** |
| **AO-022/43360684** | **-8.58**  | **-7.80**  | **-69.32**  | **48.9** | **7.94** |  |  |
| **AO-080/42479572** | **-9.19**  | **-9.73**  | **-55.01**  | **1.16** | **3.74** |  |  |
| **AO-476/42169404** | **-7.16**  | **-4.37**  | **-59.79**  | **14.86** | **3.75** |  |  |
| **AP-501/42239362** | **-6.84**  | **-7.23**  | **-53.68**  | **19.49** | **4.09** |  |  |
| **AP-501/43371956** | **-9.90**  | **-9.23**  | **-51.05**  | **7.09** | **4.1** |  |  |

Table S1. The docking scores, MMGBSA score, inhibition rate of GSK3β for the 10 tested compounds

Table S2. Similarity of 3 hit compounds to Known inhibitors (please check this table on the file of supp2\_table\_S2\_similarity\_of\_hit\_compounds\_to\_Known\_inhibitors.xlsx)