|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| **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)