**Supporting Information for Original article**

**Identification of potent CAMKK2 inhibitors by virtual screening and dynamics simulation**

Le Fu1,2 † Linan Zhao1† Meichen Liang2 Kun Ran2 Jing Fu2 Haoyu Qiu2

Fei Li2,\* Mao Shu1,\*

1School of Pharmacy and Bioengineering, Chongqing University of Technology, Chongqing 400054, China

2Qianjiang Central Hospital of Chongqing, Chongqing 409099, China

\*Address correspondence to Fei Li, 17563241@qq.com and Mao Shu, shumao@cqut.edu.cn

† Equal contribution.



**Fig. S1 The pharmacophore model for CAMKK2 selected for virtual screening.**



**Fig. S2 Visual representation of four pharmacophore characteristics and exclusion of volume constraints used in AncPhore.**



**Fig. S3 Active cavity of CAMKK2.** The parameters of the active cavity are set as follows: xmin: -31.1Å, xmax: -14.4Å, ymin: -27.4Å, ymax: -4.1Å, zmin: -20.2Å, zmax: -3.2Å.



**Fig. S4 Comparison of docking conformation and crystal conformation of CAMKK2.** Pink is the docked conformation and blue is the initial crystal conformation. The RMSD value is 0.172 Å, which proves the reliability of molecular docking.

**Table. S1** **Results of the Güner-Henry Method.**

|  |  |
| --- | --- |
| Parameter | Value |
| Total number of molecules(D) | 533 |
| Number of active molecules(A) | 12 |
| Total hits(Ht) | 16 |
| Active hits(Ha) | 12 |
| Yield of actives(Ha/Ht)% | 75 |
| Ratio of actives (Ha/A) % | 100 |
| False positives(FP= Ht -Ha) | 4 |
| False negatives(FN=A-Ha) | 0 |
| Enrichment Factor (EF) | 33.31 |
| Goodness of hit (GH) % | 80.63 |