

Supplementary Information

Legend to Supplementary Figures

Figure S1a: Ramachandran plot of PH0702.

Figure S2b: PROSA results of PH0702 modeled protein (Fig b) and Template 2YRF (Fig a)

Figure S2: RMSD (A) and RMSF (B) of PH0702 protein ligand complex during the MD simulation period of 30 ns.

Figure S3: Distribution of HOMO (A to E) and LUMO (F to J) of the five top compounds.

Figure S4: Distribution of MESP profile of top five compounds.

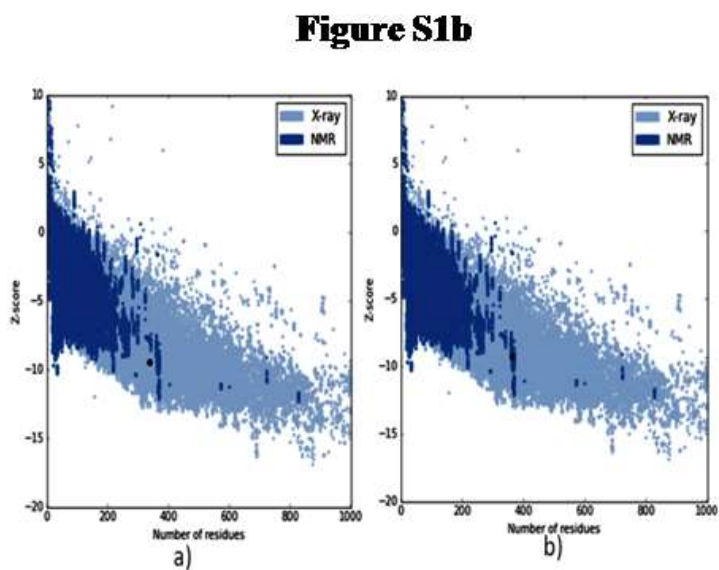
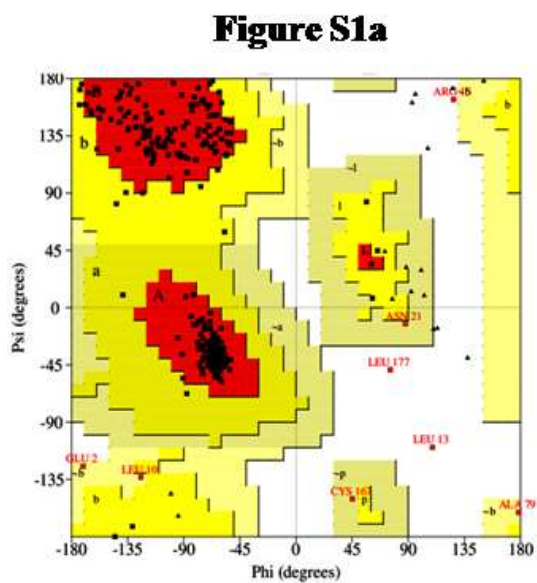


Figure S2

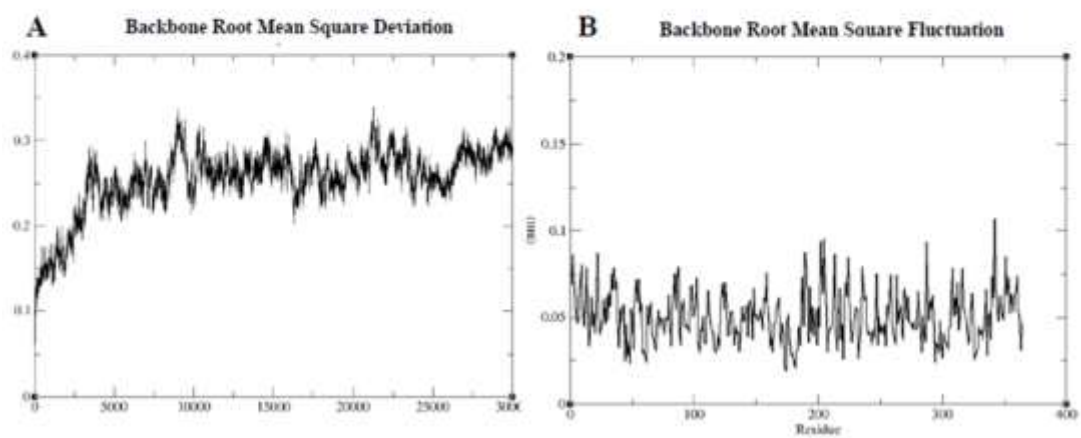


Figure S3

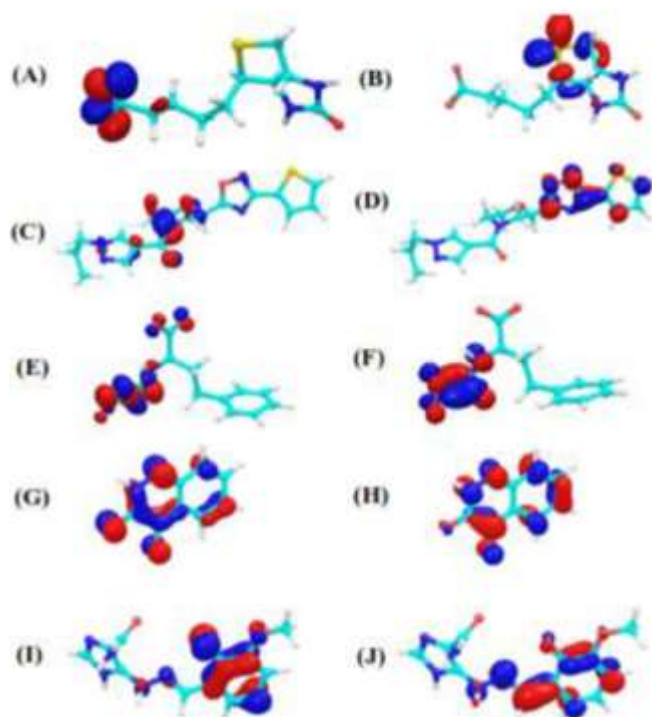


Figure S4

