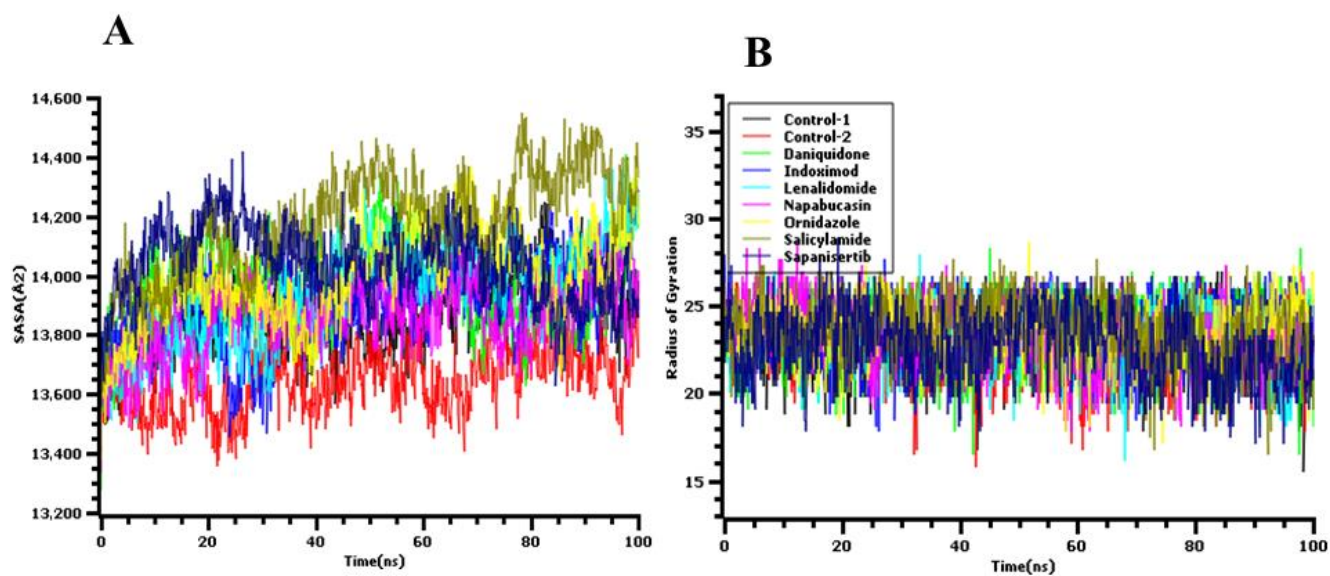


Supplementary Materials



**Figure S1.** The molecular dynamics simulation study of the docked complex, (A) solvent accessible Surface area (SASA) and (B) radius of gyration (Rg) were assessed from the simulation trajectories.