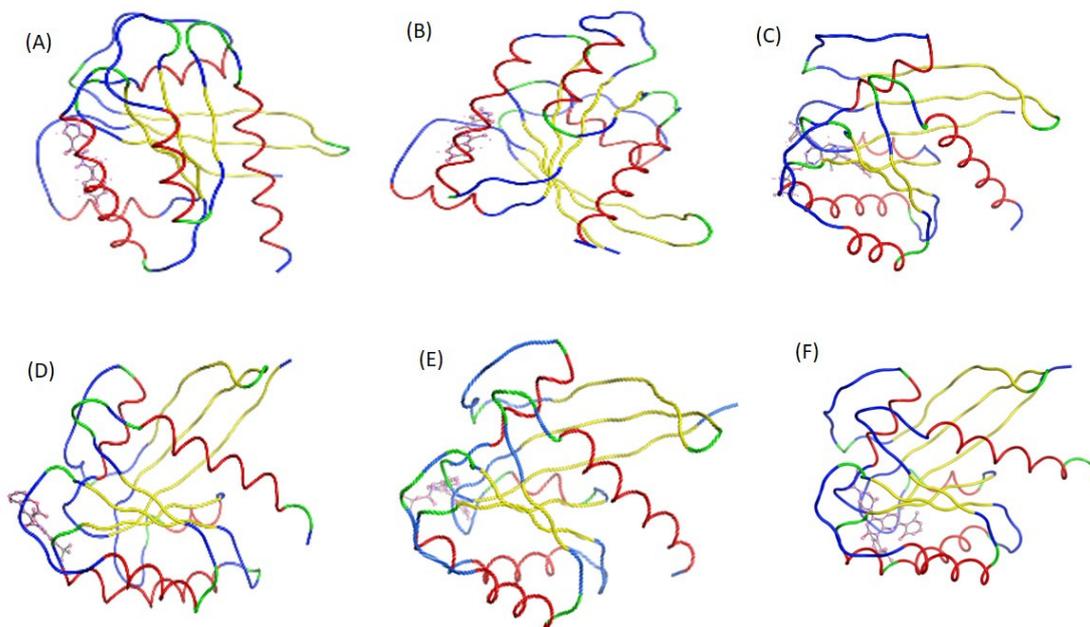


**Figure S1.** RMSD plot for ligands ZINC05524764 (Green) ZINC05828661 (Purple) and Control (Red) systems. Time in ns is shown on the X-axis and the RMSD value of each ligand is shown on the Y-axis.



**Figure S2.** (A–C) indicates the complex ZINC05524764, ZINC05828661, and Control systems before MD simulation while (D–F) indicates the ZINC05524764, ZINC05828661, and Control systems after MD simulation.