



**Figure S1 (Supplementary Figure):** Analysis of MD simulation trajectories against function of RMSD, Rg, hydrogen bond, SASA and RMSF of PLK1 (PDB ID: 2OWB) with control compound BI2536 (ligand) complex at 100000 ps (100 ns). (a) RMSD; (b) Radius of gyration (Rg); (c) Hydrogen bonds; (d) SASA; (e) & (f) RMSF plot of protein in presence of BI2536.