

Fig. S1. Monitoring the fluctuations of RMSD of the protein of backbone, residues within 5Å of binding pocket and the heavy atoms of ligand in MD simulations.

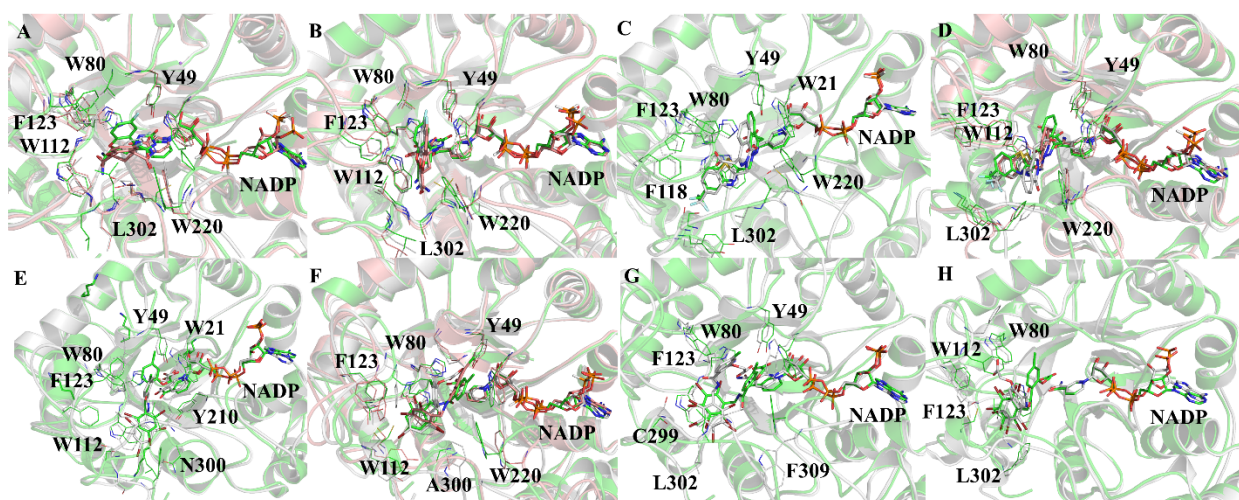


Fig. S2. Superimposition of the average structure deriving from the last 100ns in MD trajectory and the initial pose. Green cartoon represents the initial structure, red represents the structure of intermediate tense and gray cartoon represents the average structure deriving from the last 100ns in MD trajectory.