

Supplementary figure

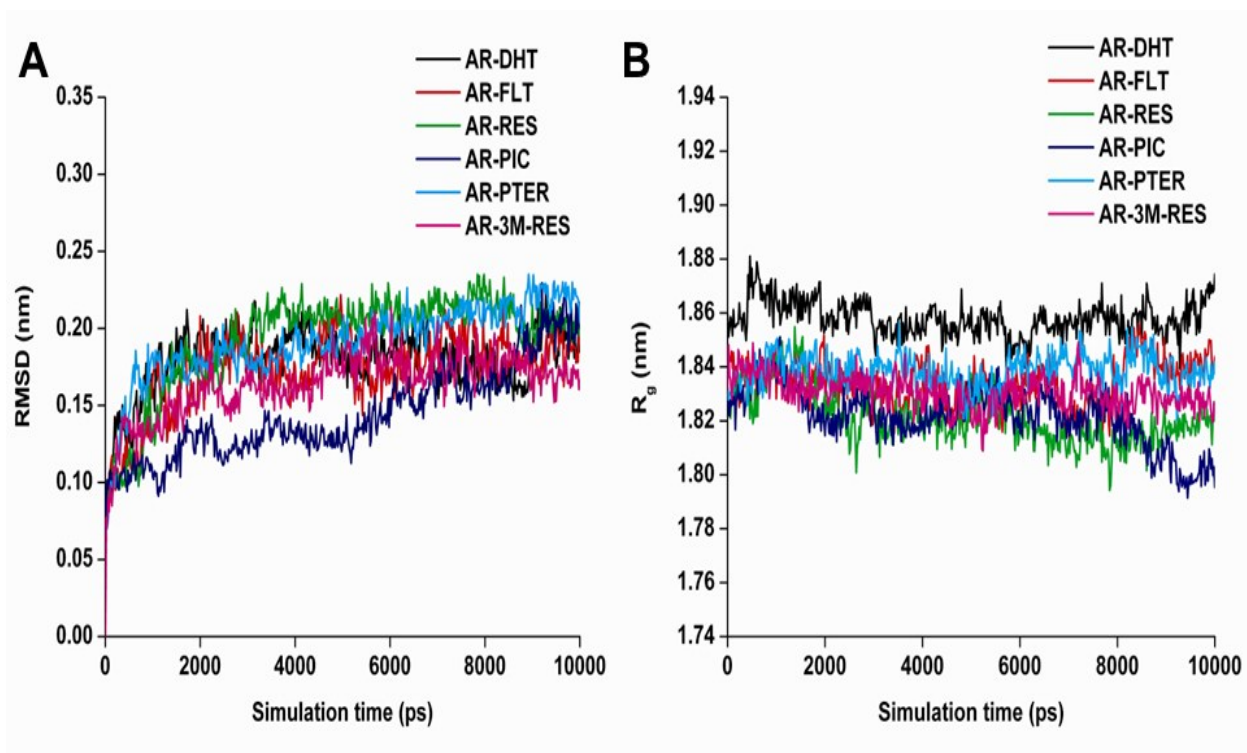


Fig. S1: Variations of dynamic parameters of AR bound to different ligands obtained from MD stimulation. (A) Variations in $C\alpha$ -RMSD of AR monomer in presence of different bound ligands with simulation time. (B) Radius of gyration R_g profile of AR-ligand complexes with simulation time.