Figure S2. Binding energy of receptor-ligand complex for the template (A) and modelled complex between Geldanamycin and swine HSP90AB1 (B) during MD simulations (10 ns). ΔE_{vdw} refer to van der Waal energy, ΔE_{elec} refer to electrostatic energy, ΔE_{mm} refer to total potential energy between the protein and ligand ($\Delta E_{mm} = \Delta E_{vdw} + \Delta E_{elec}$), ΔE_{pol} refer to polar solvation energy, ΔE_{apol} refer to non-polar solvation energy and $\Delta E_{binding}$ refer to the total binding energy ($\Delta E_{binding} = \Delta E_{mm} + \Delta E_{pol} + \Delta E_{apol}$).