Supplementary Figures

Figure S1. Contribution energy for each residue in the template (A) and modelled complex between Geldanamycin and swine HSP90AB1 (B). MM: contains van der Waals, electrostatic interactions, and net non-bonded potential energy between the protein and inhibitor; Polar: polar solvation energy; Apolar: non-polar solvation energy; Total: total energy.