S5 Fig. Backbone RMSDs as a function of time for the initial and successive structures of HER2/peptides complexes in MD trajectories. (A) HER2/4665, (B) HER2/58F, (C) HER2/63Y, (D) HER2/55V, (E) HER2/58F63Y, and

(F) HER2/55V63Y. The RMSD values become stable after about 5000ps in the MD trajectories, indicating the convergence of each peptide structure towards an equilibrium state.