



S8 Fig. Binding models of HER2/peptides complexes: 4665/HER2 (A), 58F/HER2 (B), 63Y4665/HER2 (C), 55V/HER2 (D), 58F63Y/HER2 (E), and 55V63Y/HER2 (F). Blue cartoons stand for mutant peptides. Key residues (binding free energy <-1 kcal/mol) in HER2 protein are shown as yellow sticks.