



S7 Fig. Binding free energy decomposition for key residues of the HER2 protein in the six complexes. HER2/4665 (A), HER2/58F (B), HER2/63Y (C), HER2/55V (D), HER2/58F63Y (E), and HER2/55V63Y (F). Green bars in the figure represent binding free energy <-3 kcal/mol. Therefore, each mutant shown in B to F has more than three residues that contribute to the HER2/peptide complexes.