



Figure S9: Ensemble-based Docking results performed with Autodock Vina (Vina). Histograms showing the relative frequency of the 19,119 molecules according to the Vina binding energy (kcal/mol) to E6 protein. **a)** Assay 1, conformation c. **b)** Assay 2, conformation a. **c)** Assay 2, conformation b. **d)** Assay 3, conformation a.