

Supplementary Materials

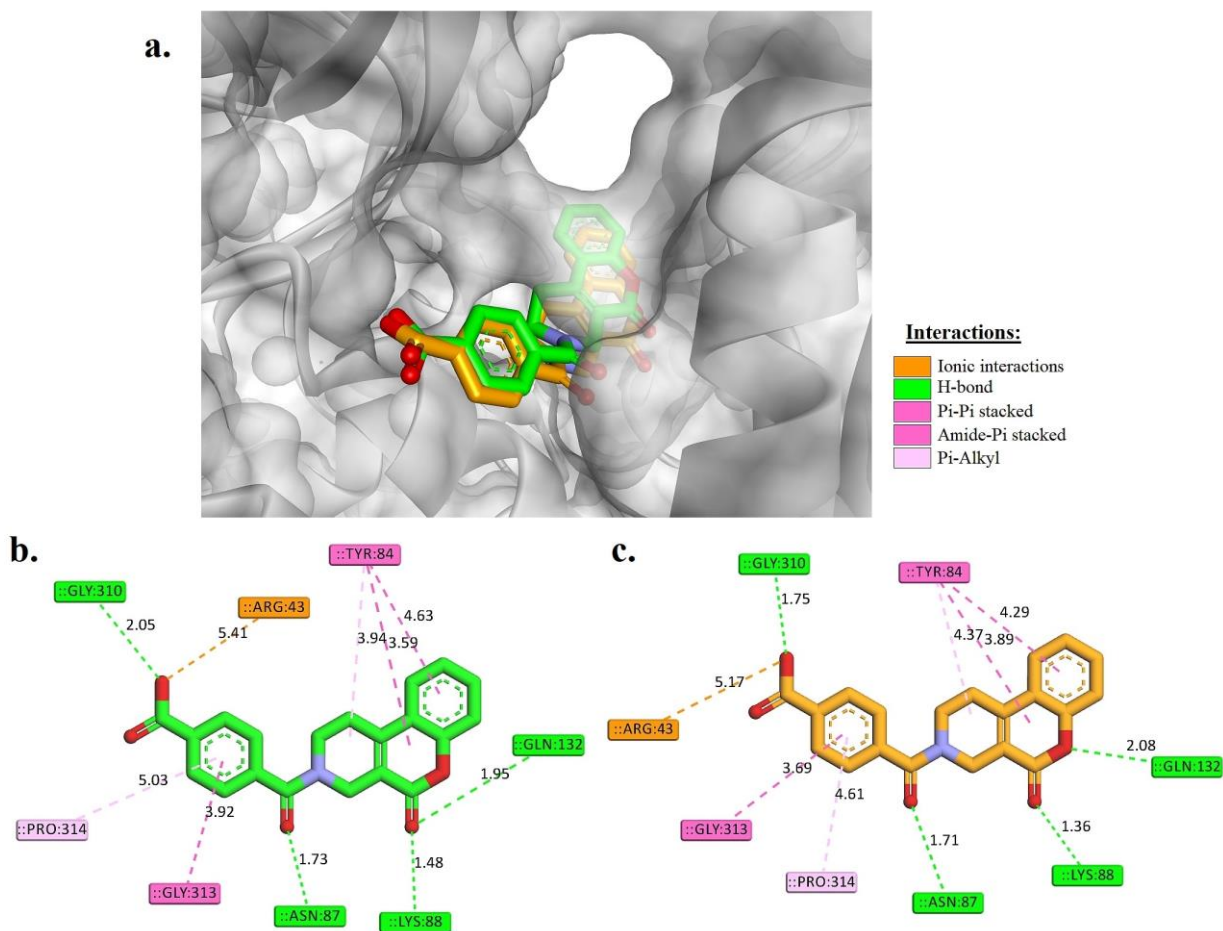


Figure S1. (a.) Superimposition and (b.) 2D interaction analysis of the co-crystallized ligand (DS44960156) (highlighted in green for carbon (C), red for oxygen (O), and navy for nitrogen (N)). (c.) Re-docked ligand (highlighted in orange for carbon (C), red for oxygen (O), and navy for nitrogen (N)) within the crystal structure of the human MTHFD2 enzyme (PDB ID: 6JIB).