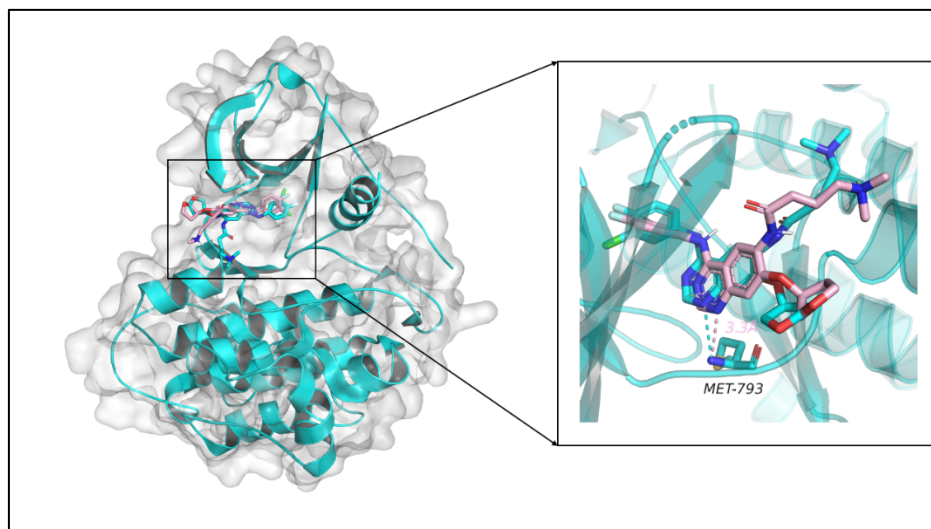
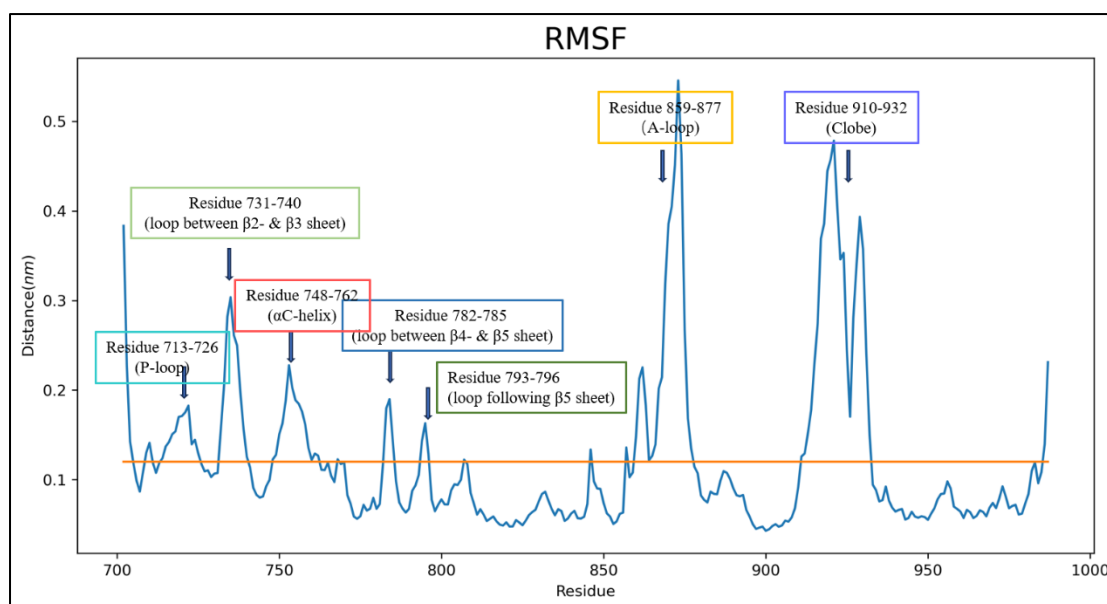


SUPPLEMENTARY INFORMATION CHAPTER 5



Supplementary Figure 1. An example of afatinib successfully redocked to the WT EGFR kinase. A validated docking pose of afatinib is depicted in light pink and superimposed with the experimental afatinib-bound WT EGFR structure, which is represented as a cyan cartoon (PDB ID: 4G5J). The hydrogen bond between afatinib and Met793 is indicated by a dotted line. An acceptable pose maintains a hydrogen bond with methionine 793 and has ligand orientation similar to the crystal structure (in RMSD of heavy atoms). A hydrogen bond was defined as a donor-acceptor distance of ≤ 3.5 Å and a bond angle between acceptor-hydrogen-donor of $\geq 135^\circ$.



Supplementary Figure 2. The Root Mean Square Fluctuation (RMSF) analysis plot illustrates the dynamic behavior of each residue within the inactive wild-type EGFR (PDB ID: 1XKK) over the course of the simulation. A horizontal line representing the average RMSF value across all residues is included for reference.