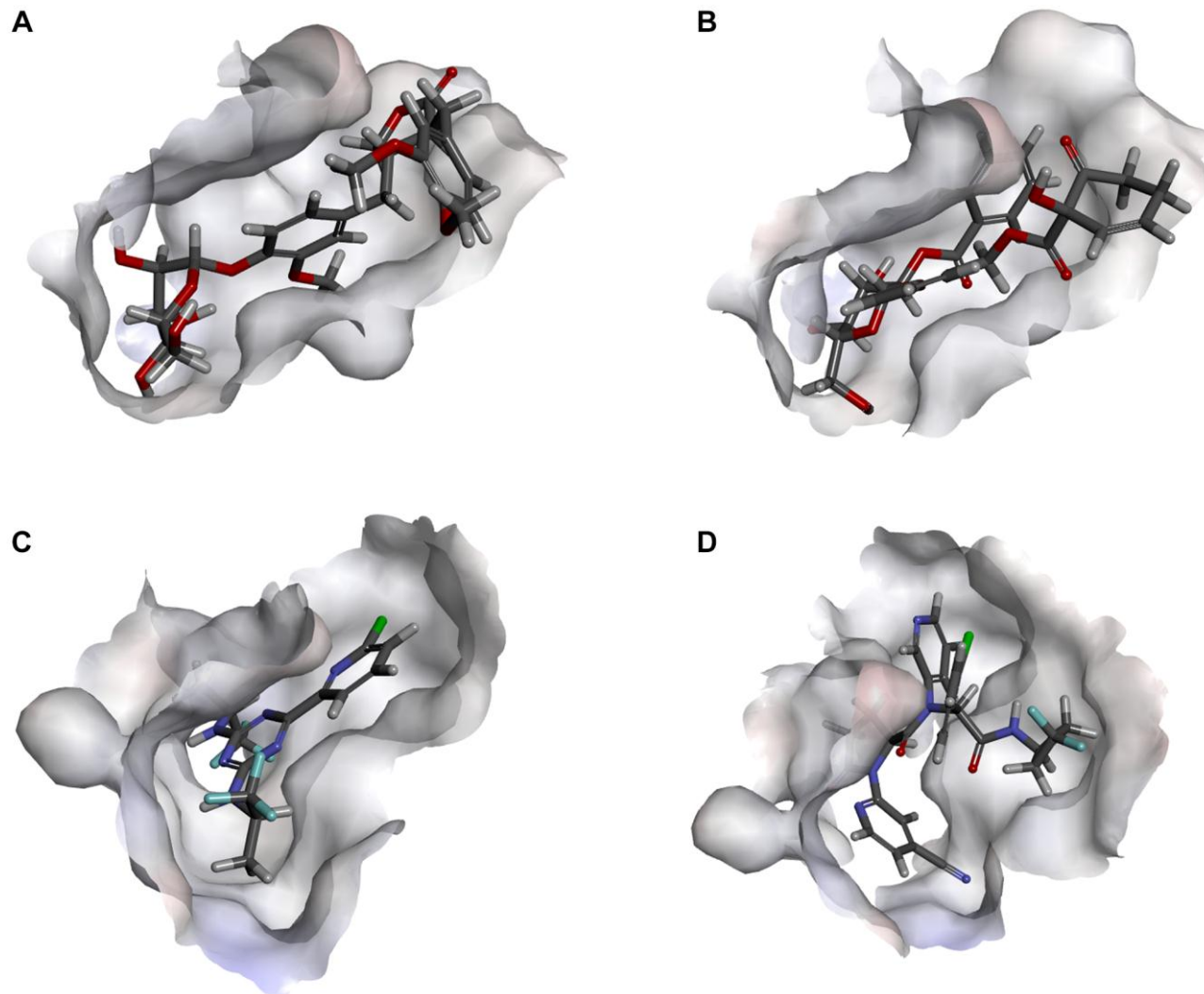


SUPPLEMENTARY FIGURE



Supplementary Figure 1. Schematic drawing of interactions between ligands and IDH1_R132H and the ionizability surface of the junction pocket was added, blue represented basic ionization, red represented acid ionization, and ligands were shown in sticks, the structure around the ligand-receptor junction were shown in thinner sticks. (A) ZINC000004098459 (B) ZINC000049872393 (C) Vorasidenib (D) Ivosidenib.