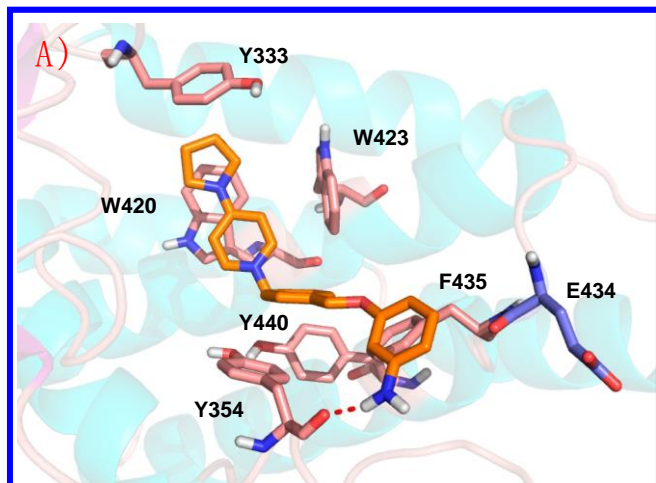
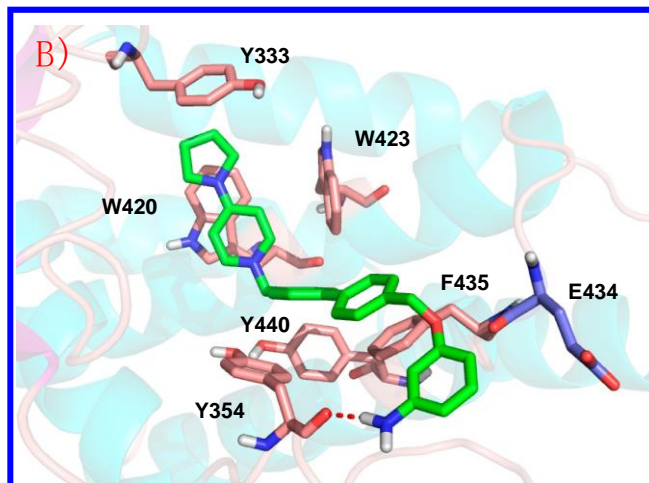


# Supplementary Materials: Anticancer and Structure Activity Relationship of Non-Symmetrical Choline Kinase Inhibitors

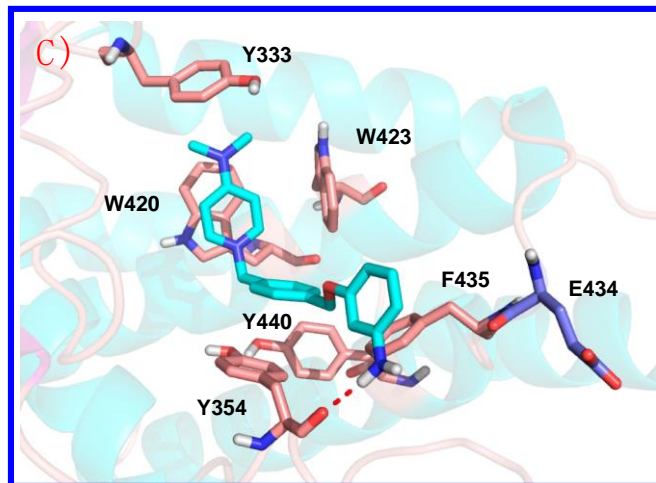
Santiago Schiaffino-Ortega, Elena Mariotto, Pilar María Luque-Navarro, María Kimatrai-Salvador, Pablo Rios-Marco, Ramon Hurtado-Guerrero, Carmen Marco, María Paz Carrasco-Jimenez \*, Giampietro Viola \* and Luisa Carlota López-Cara \*



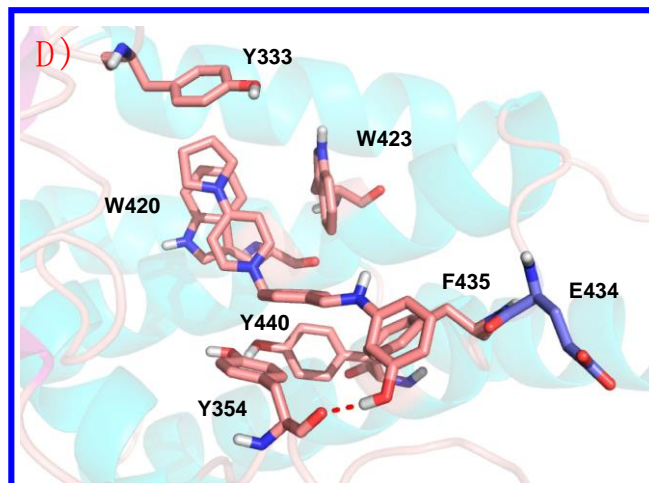
Compound 3a



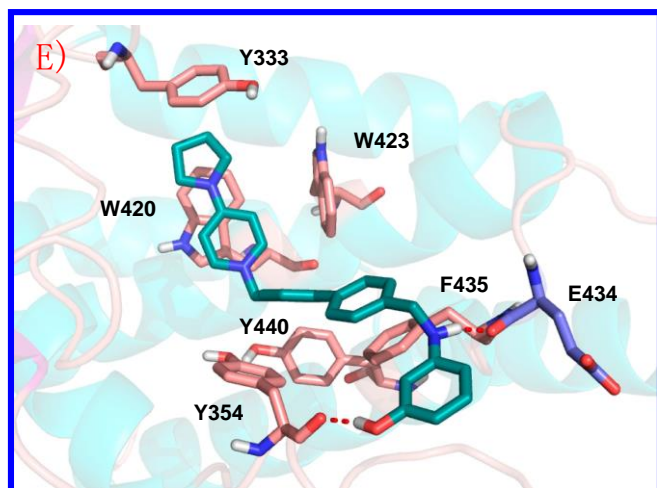
Compound 3b



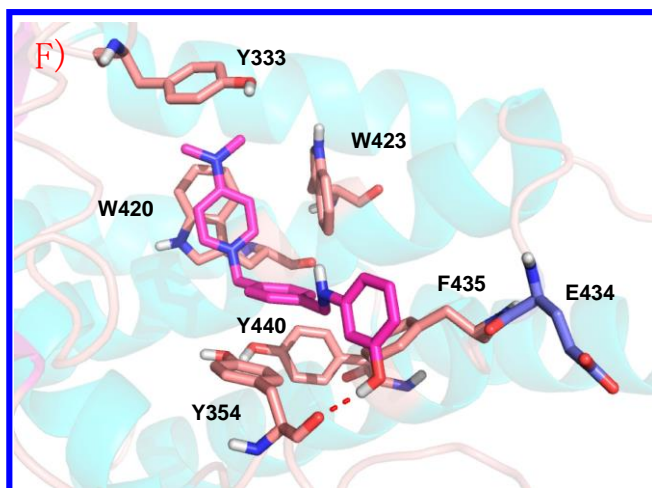
Compound 3e



Compound 4a

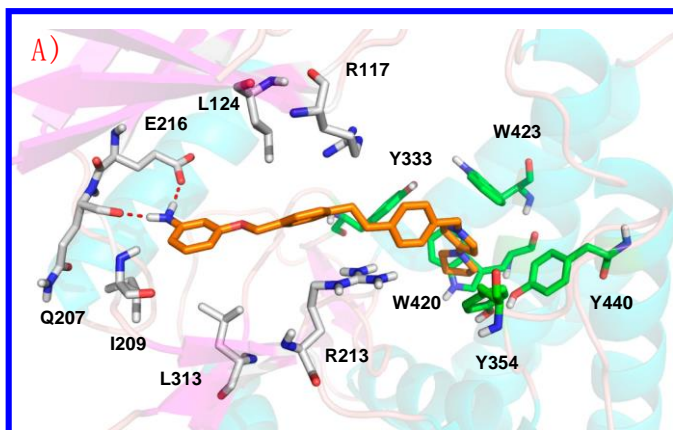


Compound 4b

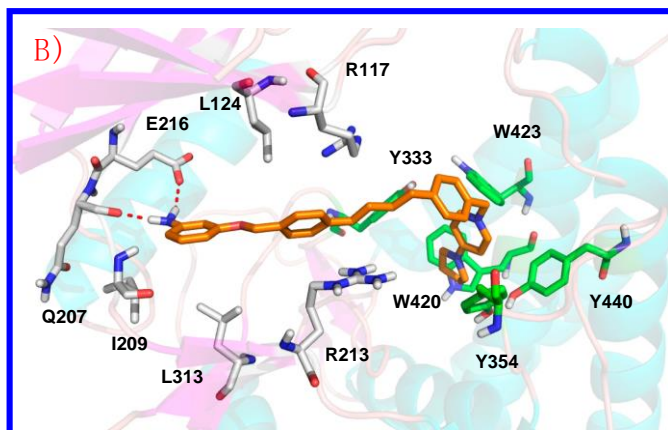


Compound 4e

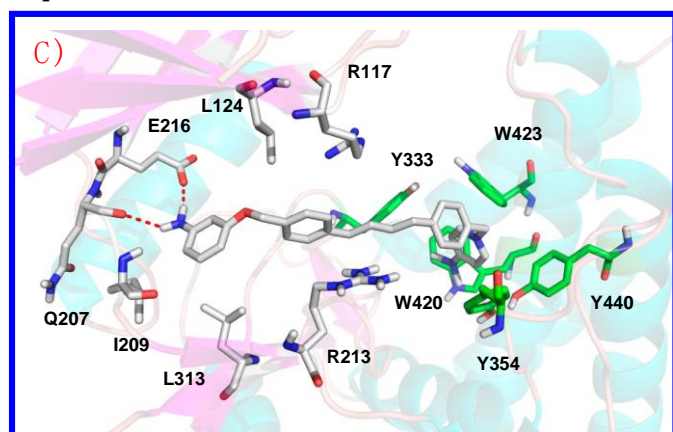
**Figure S1.** Poses obtained in the docking studies of compounds **3a** (A, carbon atoms in orange colour), **3b** (B, carbon atoms in green colour), **3e** (C, carbon atoms in cyan colours), **4a** (D, carbon atoms in salmon colours), **4b** (E, carbon atoms in slate colour) and **4e** (F, carbon atoms in magenta colour), inserted into the Cho binding site similarly to of ChoK $\alpha$ 1/6 complex (PDB ID: 4BR3).



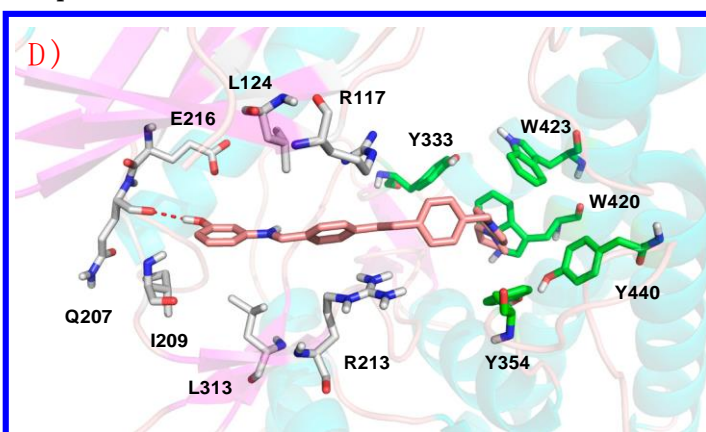
Compound 3c



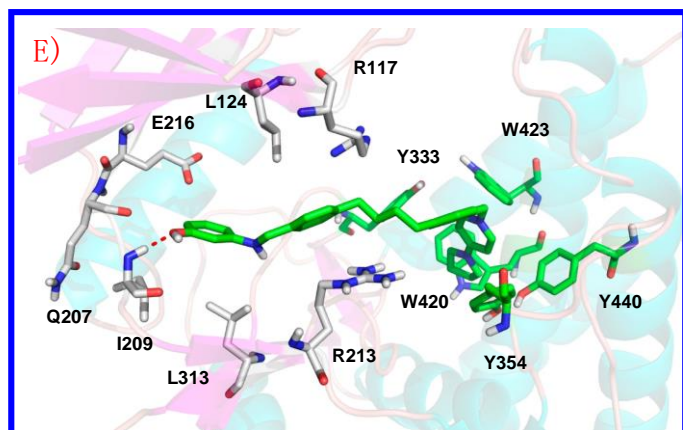
Compound 3d



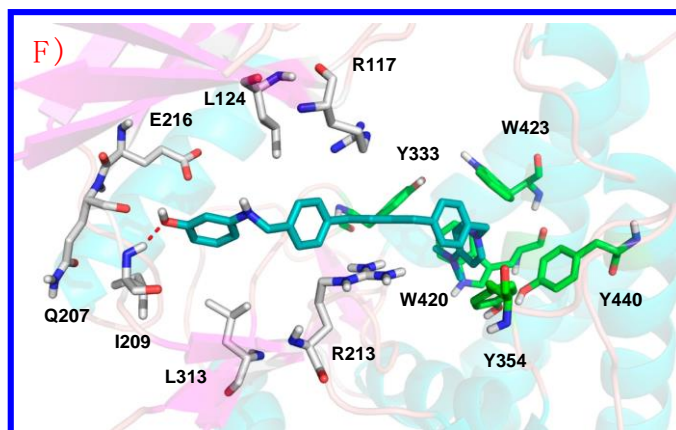
Compound 3h



Compound 4c



Compound 4d



Compound 4h

**Figure S2.** Poses obtained in the docking studies of compounds **3c** (A, carbon atoms in orange colour), **3d** (B, carbon atoms in orange colour), **3h** (C, carbon atoms in white colours), **4c** (D, carbon atoms in salmon colours), **4d** (E, carbon atoms in green colour) and **4h** (F, carbon atoms in cyan colour), inserted into the ATP and Cho binding sites similarly to ChoK-α1/5 complex (PDB ID: 3ZM9).