



**Figure S9.** Docking poses of losartan similar to the co-crystallized structures. The yellow cartoon and sticks show the co-crystallized structure of CYP2C9 WT (PDB ID 5XXI) (A) and CYP2C9 A477T (PDB ID 5X23) (B). The salmon cartoon and sticks show the best-energy docking poses of losartan in the centroid number 4 conformation of CYP2C9 WT-apo (A) and the centroid number 0 conformation of CYP2C9 mutant –bound losartan (B).