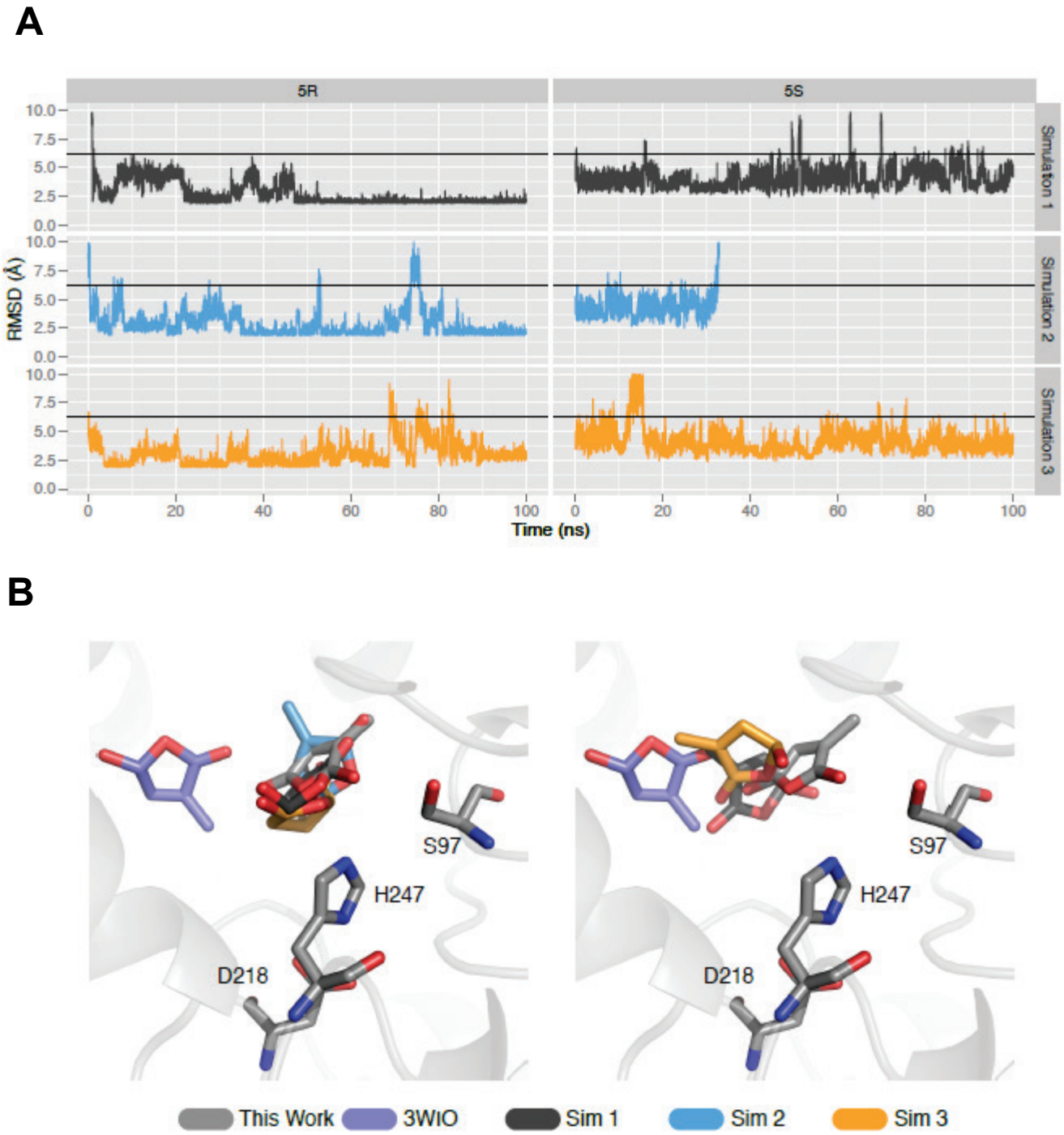

Supplementary information, Figure S12 Simulations of 3WIO D-OH stereoisomer products. (A) Root-mean squared deviation (RMSD) of 5R and 5S D-OH ligands using the position identified in this work as the reference structure. Lower RMSD values indicate binding positions consistent with the D-OH ligand identification of this work. Additionally, a horizontal line at 6.22 Å indicates the starting difference between 3WIO and this work. **(B)** Representative snapshots of 5R (left) and 5S (right) D-OH binding taken from the last frame of each simulation at 100 ns. All 5R and two 5S simulations adopt RMSD conformations within 2.2 and 3.5 Å respectively of this work. The second 5S simulation dissociates from D14 and remains in the solvent for the remainder of the simulation.