

Supplementary Figures

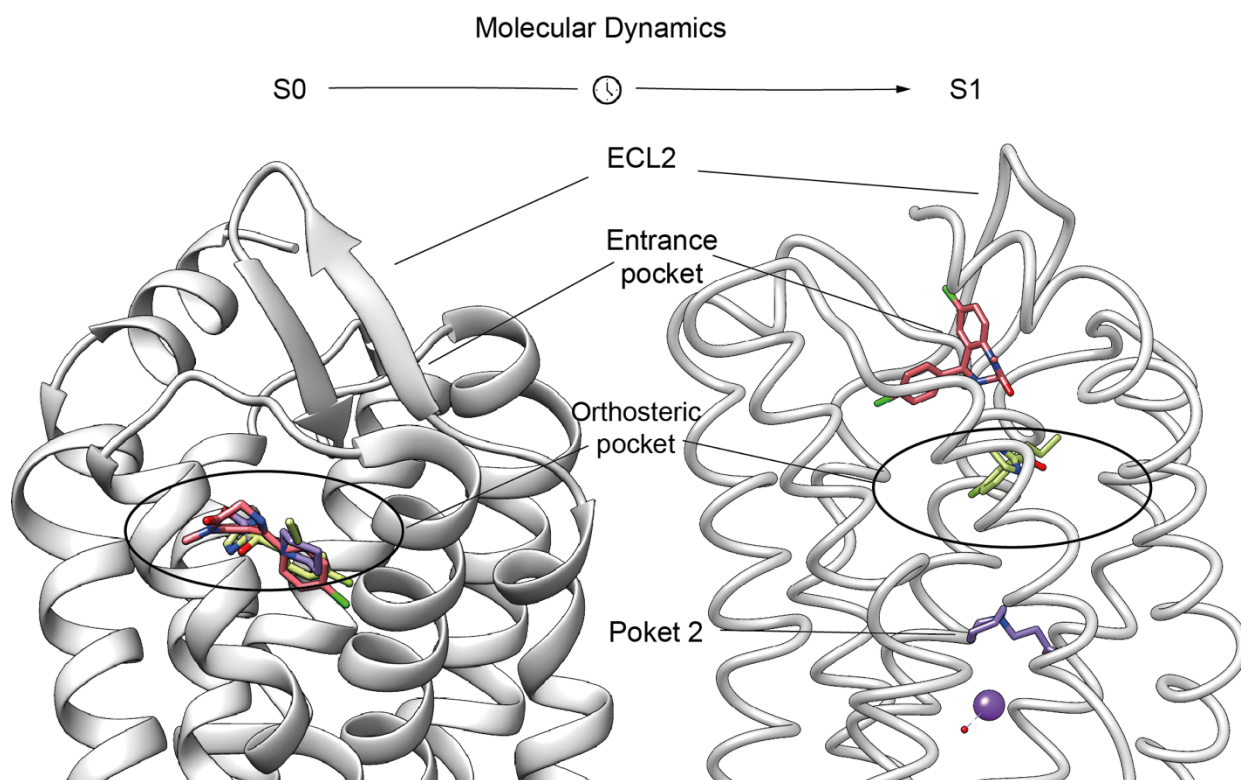


Figure S2. Movements of compounds during MD simulations. *wt*PAR2 represented in white ribbons and *wt*PAR2 white licorice respectively for the Initial State (S0) and Final State (S1) shown obtained from the Molecular Dynamics simulations. Orthosteric pocket is circled in both the structure. AZ8838 (green) shows no movement from the orthosteric pockets throughout the simulation. 1-PPA (purple) and Ro5-4864 (pink) move from the pocket with divergent directions: 1-PPA gets engulfed in the allosteric pocket, otherwise Ro5-4864 moves towards the extracellular space.