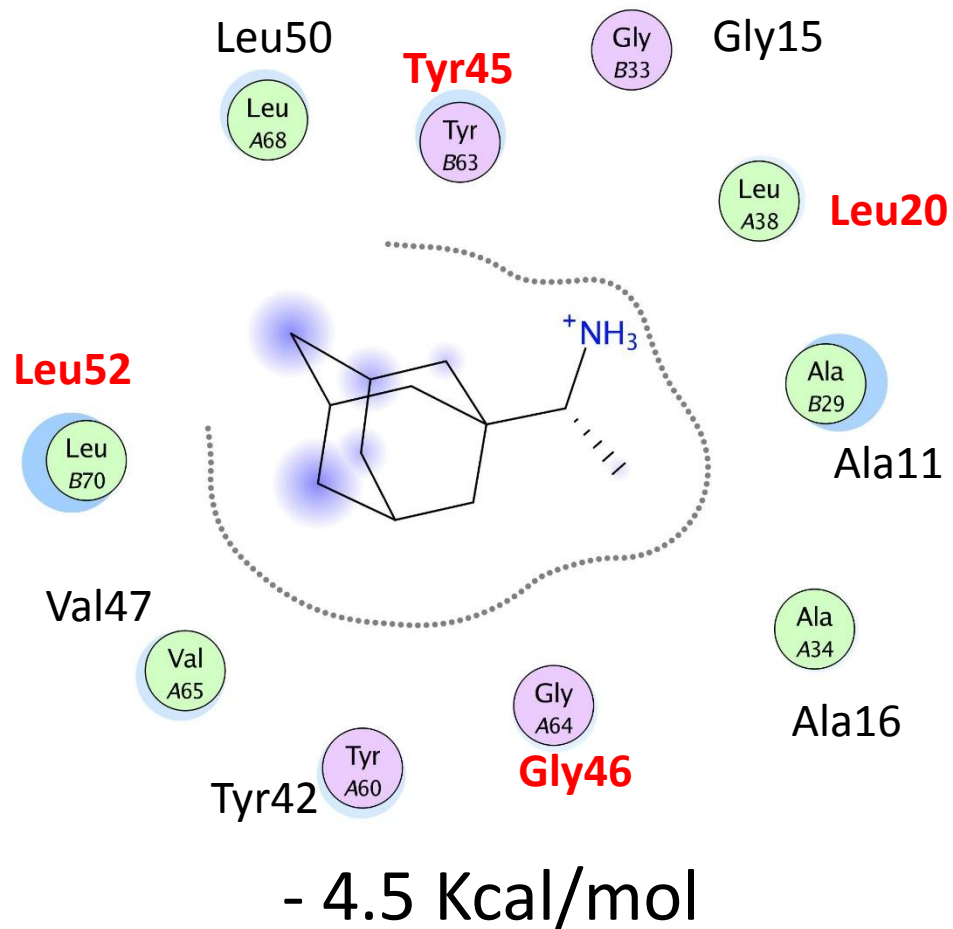
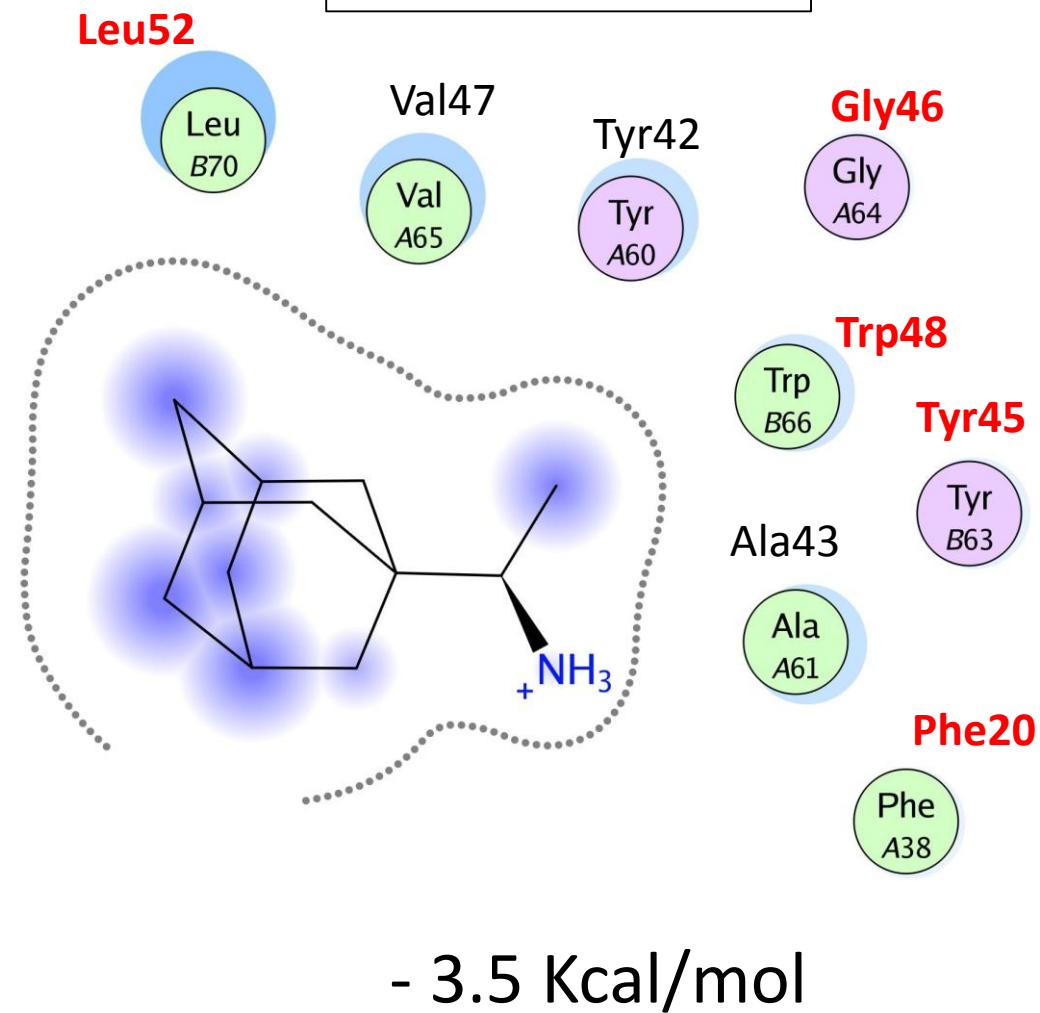


Wild-Type



L20F Mutation



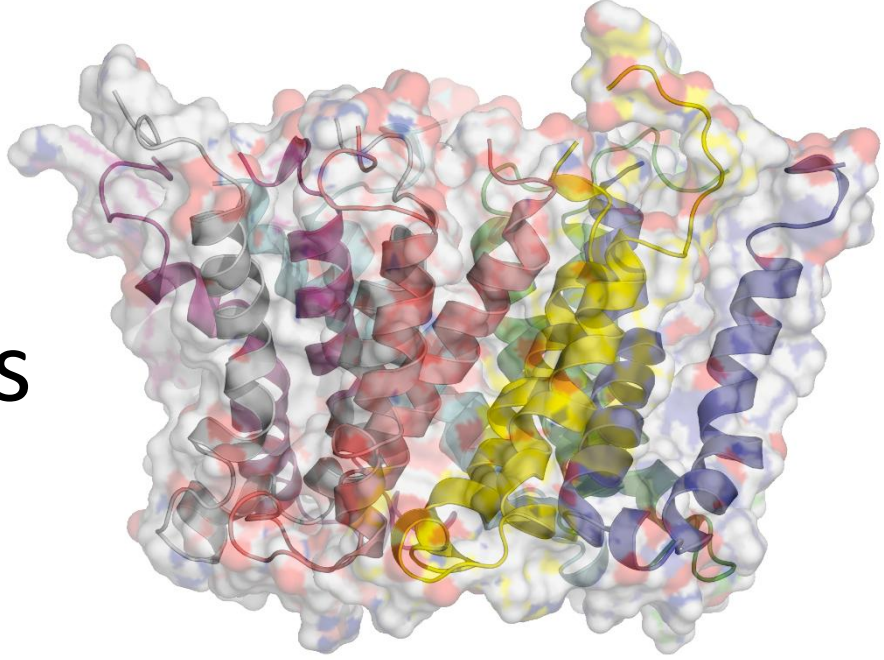
- | | | | |
|---------------------|----------------------|---------------------|-----------------|
| ○ polar | → sidechain acceptor | ○ solvent residue | ⊞ arene-arene |
| ○ acidic | ← sidechain donor | ○ metal complex | ⊞H arene-H |
| ○ basic | → backbone acceptor | → solvent contact | ⊞+ arene-cation |
| ○ greasy | ← backbone donor | → metal/ion contact | |
| ○ proximity contour | ● ligand exposure | ○ receptor exposure | |

Simulation Results

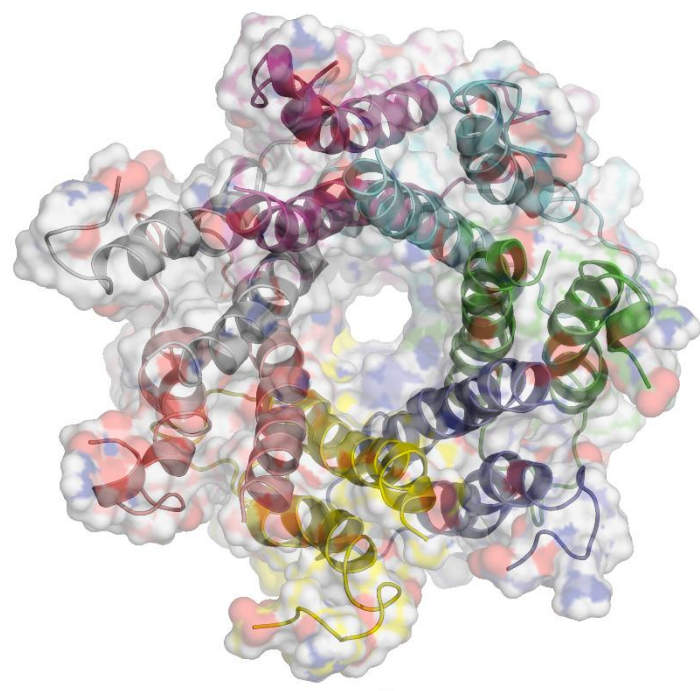
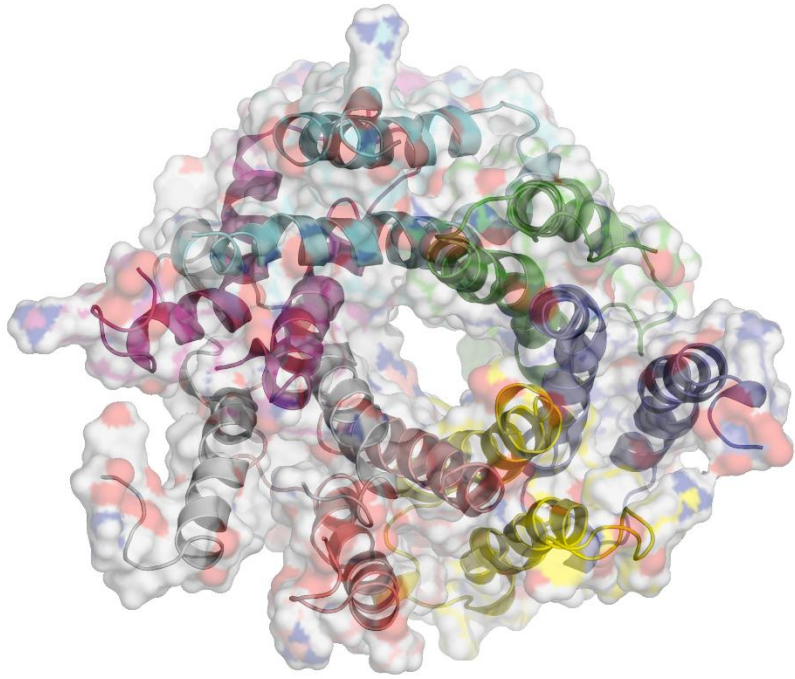
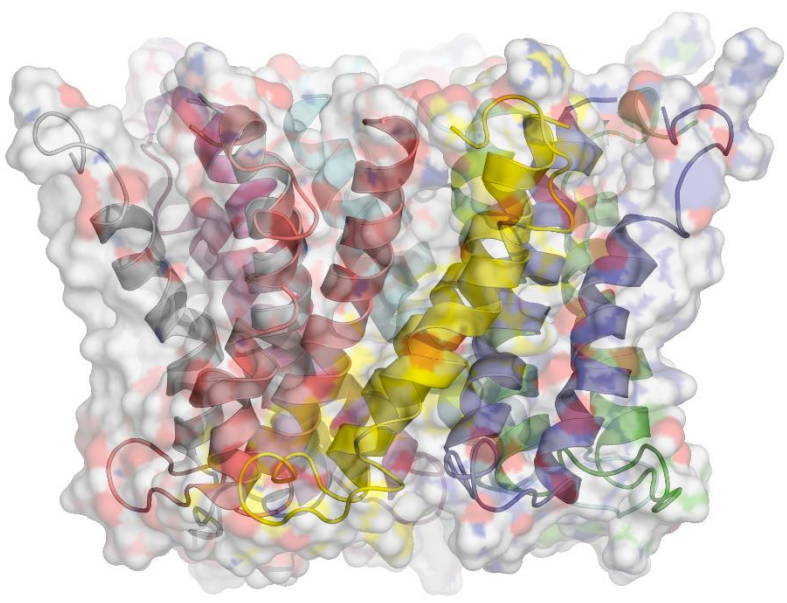
All the simulations were carried out for 100ns. A blank simulation was carried out without any ligand docked into it.

Wild type protein

100ns



0ns

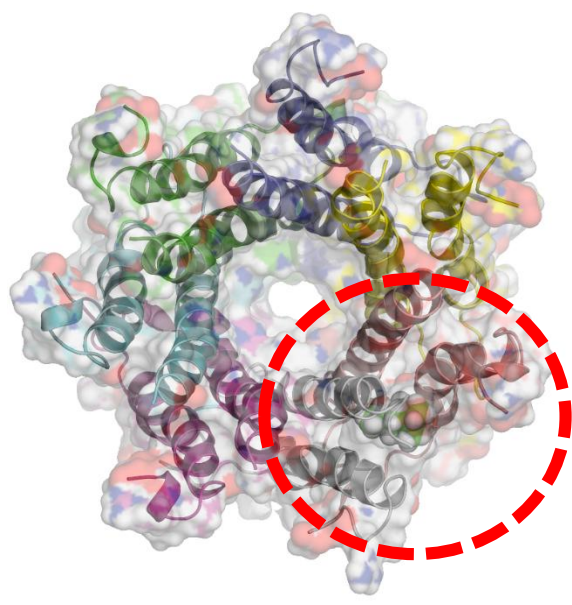
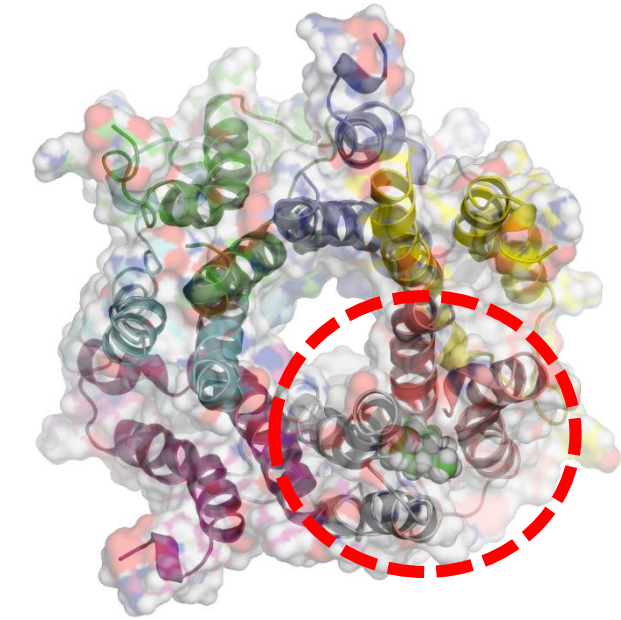
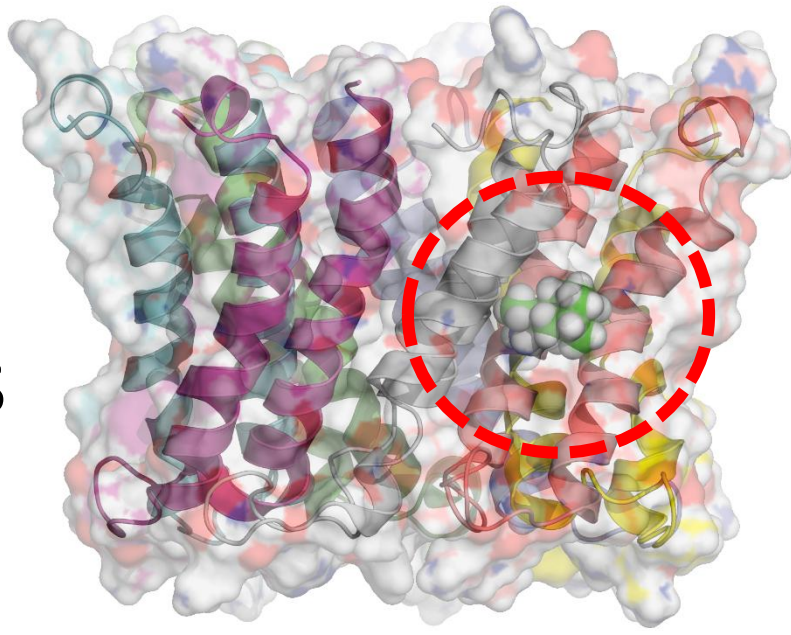
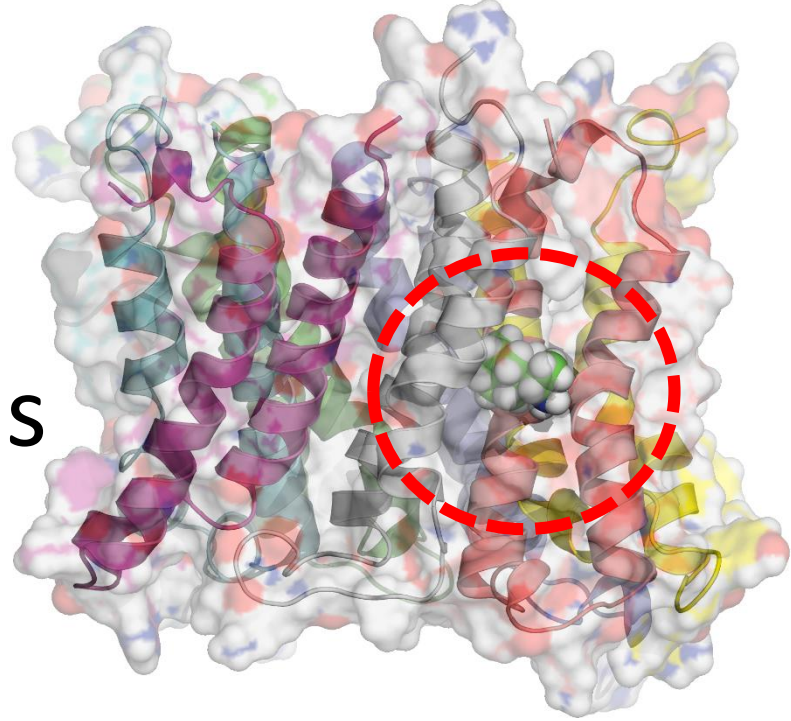


Protein without any ligand

Wild type protein

100ns

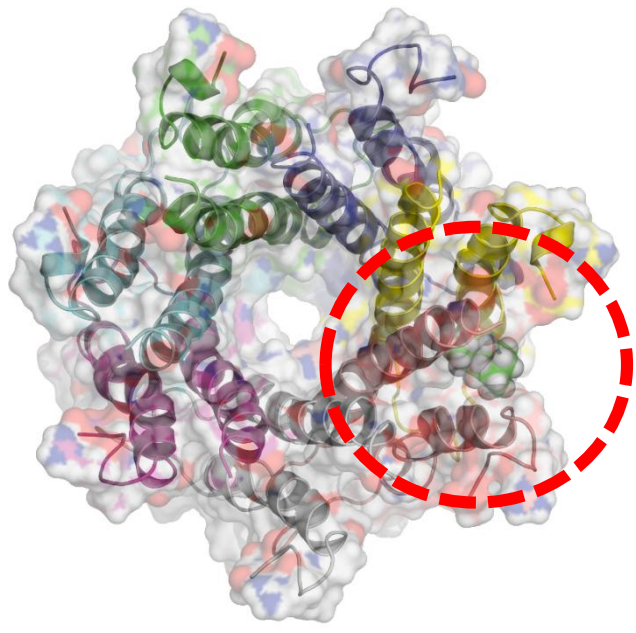
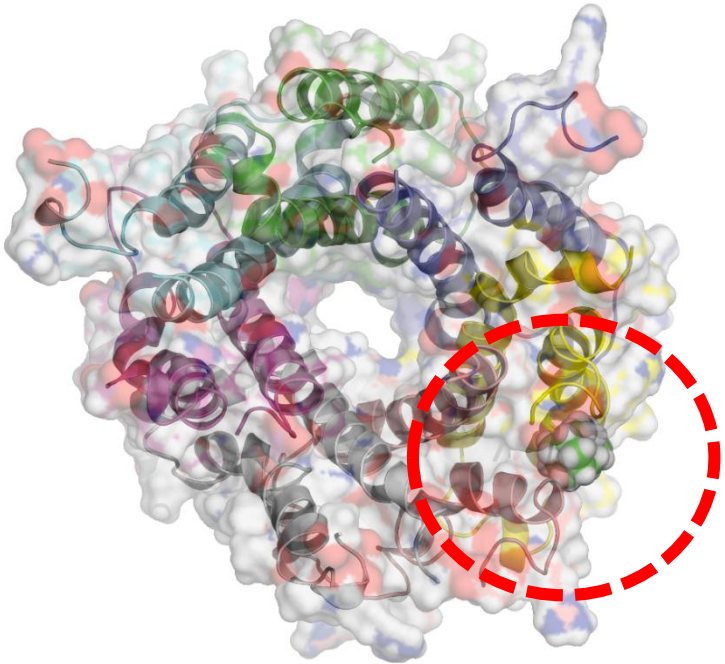
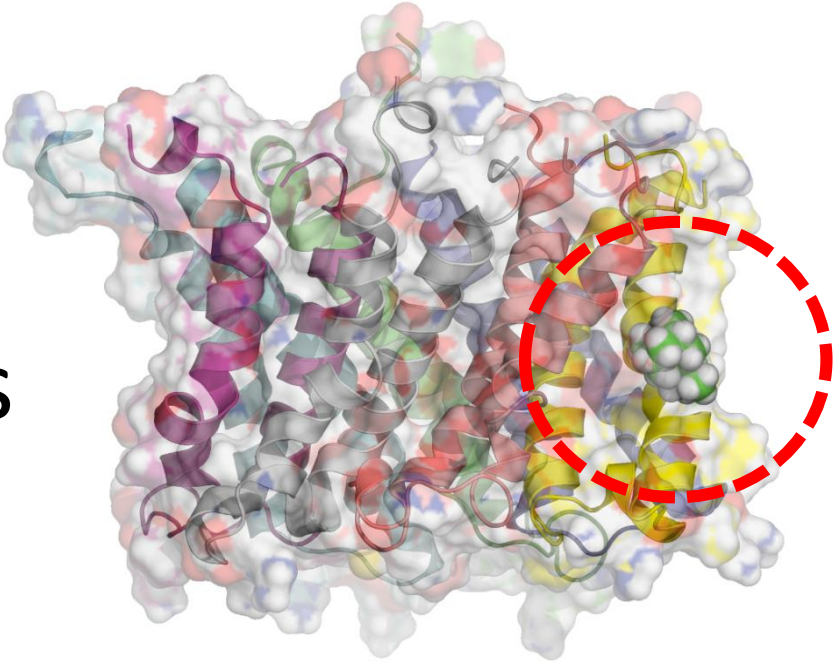
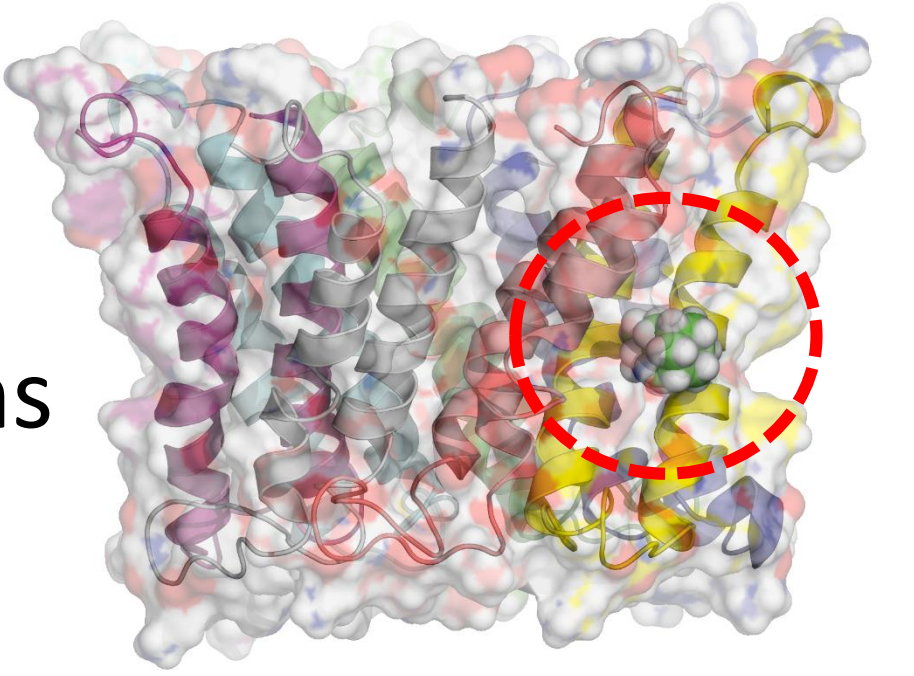
0ns

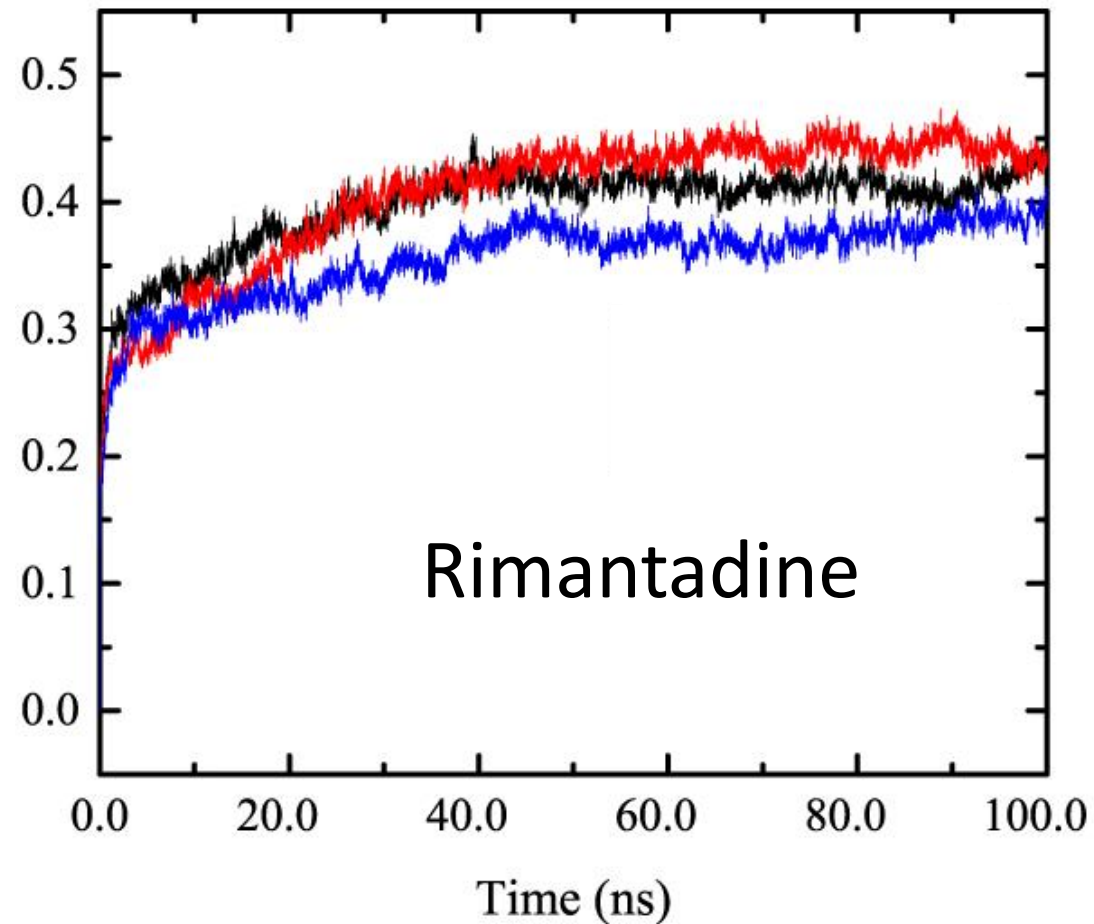
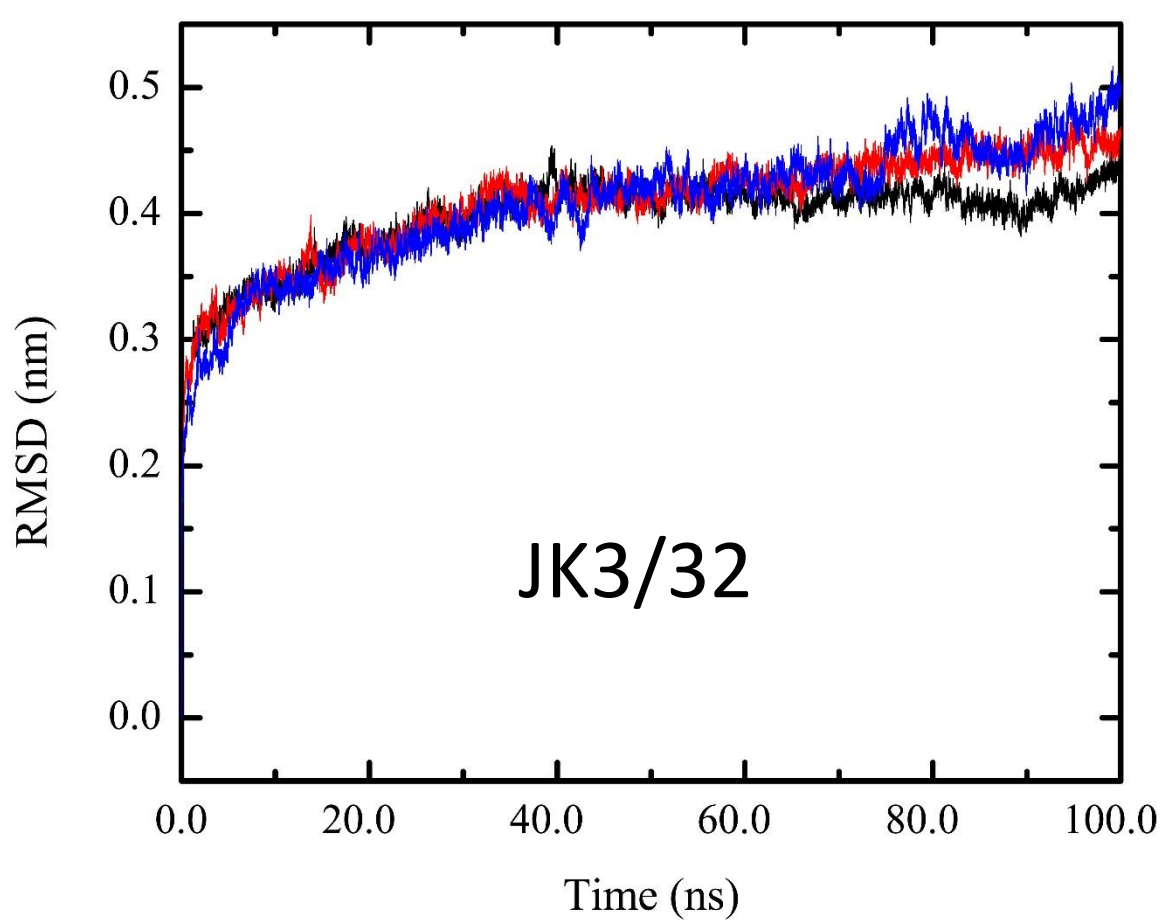


Protein with Rimantadine

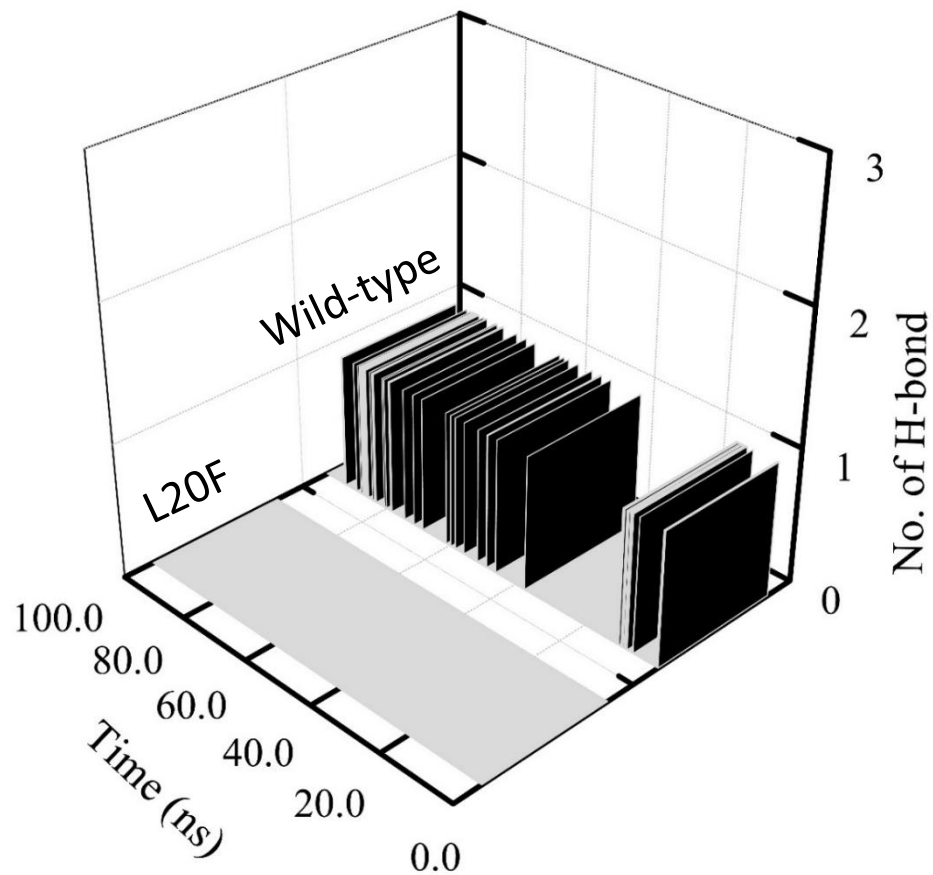
100ns

0ns

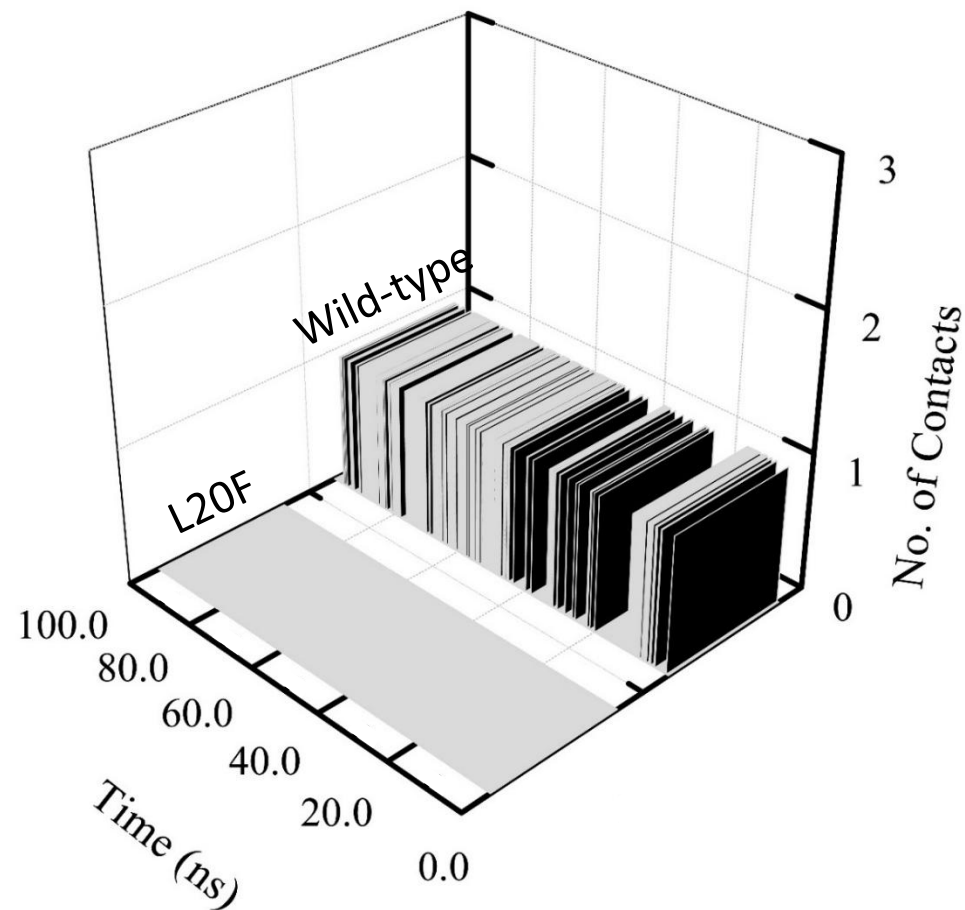




Plot of RMSD values over time for protein without any ligand (**black line**) and with ligand (wild-type: **red line**, L20F mutant: **blue line**)



This figure describes the number of H-bonds between the ligand and the side-chains of the protein over the course of simulation



This figure describes the number of contacts (but not bonding) made within a range of 3.5 Å between the ligand and the side-chains of the protein over the course of simulation

From the simulation over 100ns it is evident that only in the **wild type** of the protein, the ligand makes H-bondings and contacts whilst it doesn't in **L20F mutant**. Moreover, in the **wild type**, JK3/32 is in partially continuous H-bonding with the side chains.