

Supplementary file

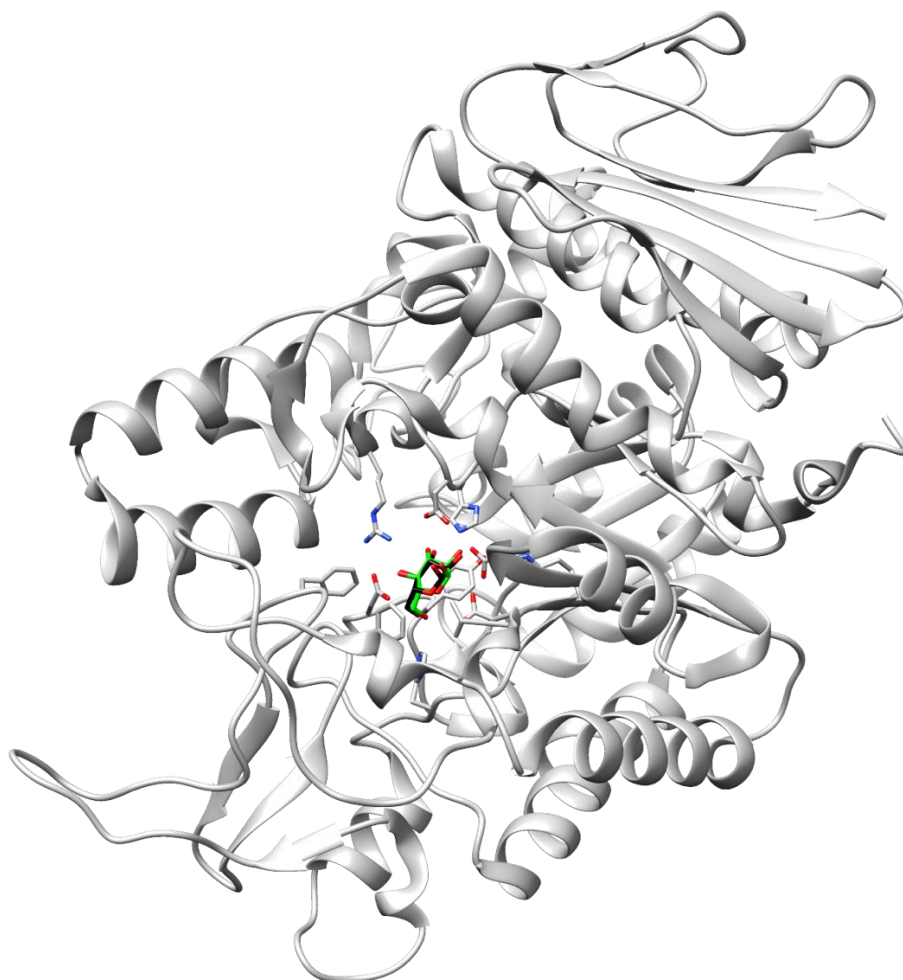


Figure S1. Molecular docking validation outcome from the established docking protocol used in this study. The RMSD value of the redocked ligand, in black, is 2.288 Å compared to the ligand's original pose (co-crystal structure position), presented in green. The accepted criterion for redocking validation is a distance of less than 3 Å.