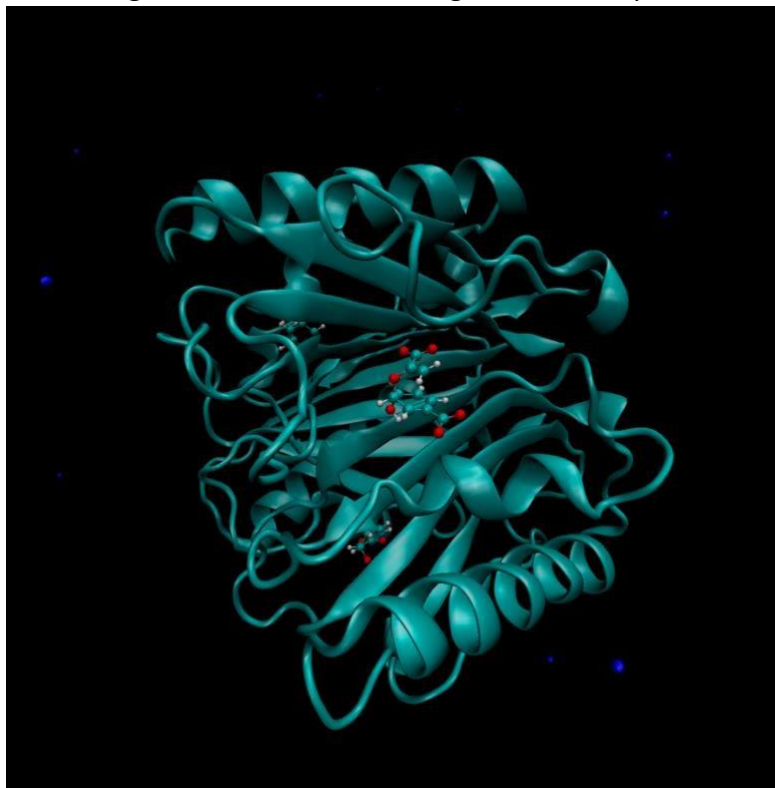
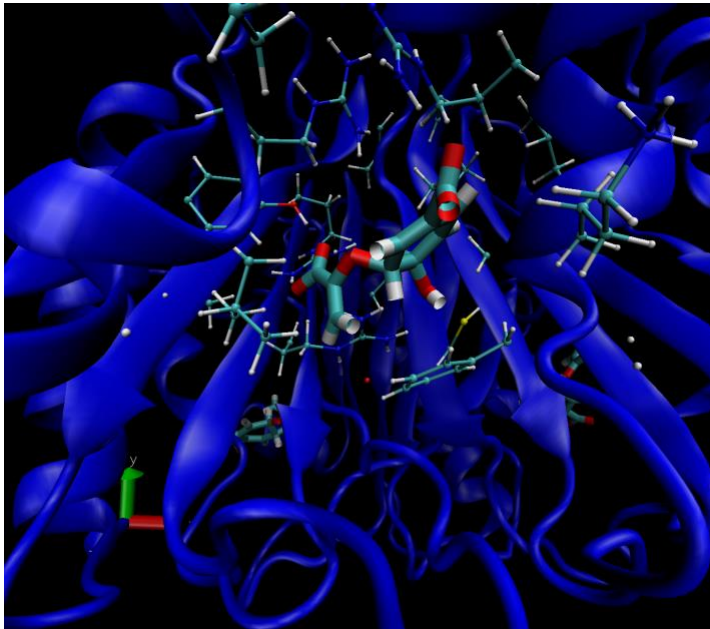


The one right in the middle is the ligand treated quantum mechanically



Before Reaction



After Reaction

