Glycoside hydrolases, also named glycosidases (GHs), are enzymes responsible of processing carbohydrates by hydrolyzing their glycosidic bond linkages. These enzymes operate either by retention or inversion of the configuration of the anomeric carbon. Generally speaking, two carboxylate-based protein residues, which perform the functions of acid/base and nucleophilic catalysts, are directly involved in the reaction. In this project, the active site of a bacterial *endo*-β-1,4-mannanase of GH family 134 will be studied by computer simulation to understand how the protonation state of these two carboxylate residues can impact the structure and dynamics of the enzyme. In addition, the configuration of the cleaved sugar ring during the simulation will be mapped.
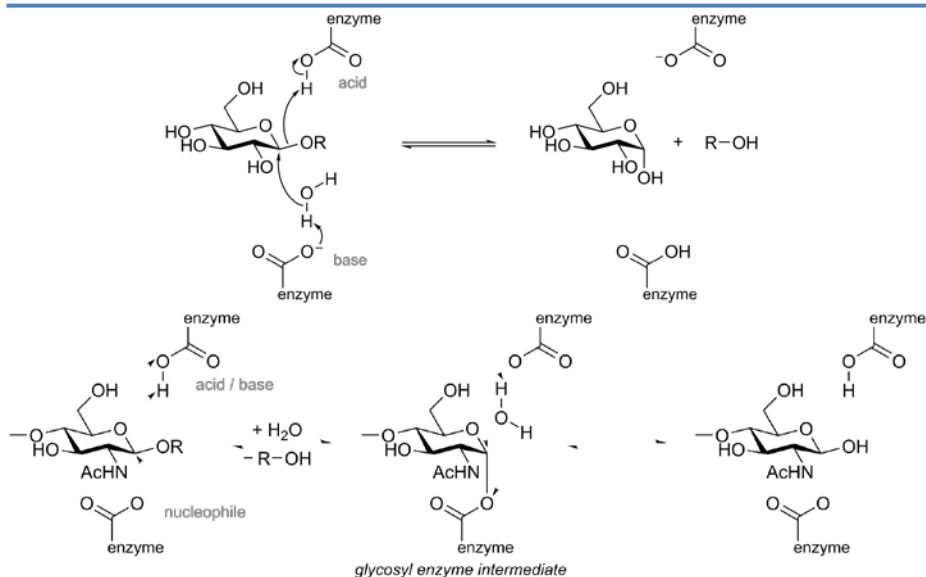
GH's mechanisms

Keywords: Computational study, Glycoside hydrolases, Sugar conformation, Carbohydrates