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**Structure characterization and molecular docking studies of α-amylase family-13 glycosyl hydrolases from Lactobacillus plantarum complexed with maltoheptaose: A novel feature of α-amylase catalytic mechanism**

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**Abstract**
The aim of the work was to contribute to the understanding of the roles played by specific binding interactions and electrostatic effects of the catalytic sites of α-amylase from Lactobacillus plantarum, which reacts with maltoheptaose. The α-amylases (E.C.3.2.1.1) from glycoside hydrolase family 13 (GH13) are one of the most important and oldest industrial enzymes. Amylases are enzymes which hydrolyze the starch molecules into polymers composed of glucose units. Although amylases be derived from several sources, including plants, animals and microorganisms. However, enzymes from fungal and bacterial sources have dominated applications in industrial sectors. Amylolytic lactic acid bacteria (ALAB) utilize starchy biomass and convert into lactic acid in single step fermentation. Only minority of lactic acid bacterial species have the capacity to produce hydrolysis enzymes. A strain L. plantarum was found to produce amylase enzyme. The results indicated that homology based approach for predicting the three dimensional (3D) structures of α-amylase from L. plantarum using α-amylase Amy 2 as start structure as templates showed a very similar structure as expected from the high sequence identity. Moreover alignment studies raised amino acid substitutions in α-amylase from L. plantarum compare to α-amylase from Bacillus subtilis which may affect the α-amylase putative active site leading to the formation of an extra hydrogen bond between Asp171, Glu200, Asp277 and Asp176, Gln 208, Asp269, respectively. The interactions between α-amylase from L. plantarum and maltoheptaose were predicted by flexible docking including minimization. Further investigations are underway to explore the positions binding site of α-amylase complexed with maltoheptaose.

**Author Keywords**
α-amylases; Family 13 of glycoside hydrolase; Homology modeling; Lactobacillus plantarum; Molecular docking

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