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Molecular Dynamics Simulation of Beta-Glucosidase of Streptomyces

Authors : Adam Abate, Elham Rasti, Philip Romero

Abstract : Beta-glucosidase is the key enzyme component present in cellulase and completes the final step during cellulose hydrolysis by converting the cellobiose to glucose. The regulatory properties of beta-glucosidases are most commonly found for the retaining and inverting enzymes. Hydrolysis of a glycoside typically occurs with general acid and general base assistance from two amino acid side chains, normally glutamic or aspartic acids. In order to obtain more detailed information on the dynamic events origination from the interaction with enzyme active site, we carried out molecular dynamics simulations of beta-glycosidase in protonated state (Glu-H178) and deprotonated state (Glu178). The theoretical models generated from our molecular dynamics simulations complement and advance the structural information currently available, leading to a more detailed understanding of Beta-glycosidase structure and function. This article presents the important role of Asn307 in enzyme activity of beta-glucosidase

Keywords : Beta-glucosidase, GROMACS, molecular dynamics simulation, structural parameters
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