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Molecular Dynamics Simulations of a new family of Glycoside Hydrolase (GH-X)

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Abstract:
Glycoside Hydrolases (GH) are enzymes that play important roles in the hydrolysis of glycosidic bonds during the degradation of biomass incomplex sugars such as cellulose, hemicellulose and amylases [1]. Consequently, the structural characterization of these enzymes is considered highly valuable for the second generation ethanol processes due to the close relationship with the sugar degradation process [2]. The use of molecular dynamics techniques to study the properties of the substrate and the catalytic residues have been essential to determine enzymatic properties that cannot be easily or impossible to study from in vivo or in vitro experimental methodologies [3]. In this study, molecular dynamics simulations were performed in order to obtain trajectories and evolution of the residues that form the catalytic side of a new glycoside hydrolase family (GH-X).

Key-words: Molecular Dynamics, Glycoside Hydrolases, Trajectories.
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