Docking and Molecular Dynamics of Glycosyl Hydrolases from *Achatina fulica's* Metagenome to 2G Ethanol Production

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Sugarcane processing results in great accumulation of biomass with high energy content, which is subject to forage and burns, generating harmful impacts on the environment. This biomass consists of cellulose (45-55%), hemicellulose (20-25%) and lignin (18-24%), and is being highly explored in obtaining 2G ethanol. One of the main obstacles for this conversion is the efficient deconstruction of the cellulose fiber, and in order to meet this demand, research is under development involving lignocellulolytic enzymes, such as glycosyl hydrolases (GH). The metagenome of african snail's gastric juice revealed sequences of GH that were identified and sequencially and functionally annotated. The interaction with substrates, 1-6 glucose residues (GR) or xylose residues (XR), was predicted by molecular *docking,* 50x88x50 and 76x76x76 grid centered on the binding site, using AutoDock and molecular dynamics (MD) simulations in a periodic water box, for 50 ns, 1 atm, 303 K, NPT by AMBER14. The tools BLAST, UniProt, KEGG and Modeller were used to study the sequences and build the three-dimensional models of endoglucanase (GH8, EC:3.2.1.4, C93%/I81%) and B-D-Xylosidase (GH43, EC:3.2.1.37, C99%/I87%) using 1WZZ (C96%/I38%) and 2EXJ (C99%/I55%) as structural templates, respectively. The binding sites were properly mapped and models validated by Ramachandran plot, RMSD and DopeScore. Docking showed good interactions with GH8 2-5GR, sugars with 6RG have docked improperly. For GH43, occurred only docked with 2-3XR due to the small size of the site. MD simulations showed stability models with respect to the templates during the entire simulation to GH8 and from 30ns to GH43, both Apo enzymes and in complexes with the best sugars found in the docking, based on RMSD and calculated B-factor. Due to optimistic results *in silico*, the perspectives include cloning of enzymes, extraction, purification, and experimental tests of activity on the cellulose fiber.

Keywords: ***Biofuels*, *cellulase*, *metagenome.***

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