

عنوان مقاله:

In silico study on the effects of Glucosamine group on Thermal Stability Of Yarrowia lipolytica Lip2 lipase

محل انتشار:

بیستمین کنگره شیمی ایران (سال: 1397)

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خلاصه مقاله:

High secretion levels of Yarrowia lipolytica developed it to a potential host for proteins production is one of the main enzymes which plays a significant role with various applications, including detergent, food, cosmetic, pharmaceutical and environmental industries [1]. Lip2, the only extracellular lipase of this yeast, is a glycosylated protein with 301 amino acids have several disulfide bonds. The crystal structure confirmed the two glycosylation sites at N113 and N134. Lip2 could have activities at low temperatures about 5°C and is rapidly deactivated over 50°C, with an optimal temperature of 37°C. Therefore, here for determining the effect of sugar moieties on Lip2 thermodynamic undergo scrutiny a comprehensive explanation the entire protein structure with its glycoside groups was assigned. In this study, MD simulations were performed by GROMACS software, version 5.1.4 [2], with the CHARMM 36M force field, in three functional temperatures of 300, 310, and 333 K for 20 ns long as production run. Regarding to the results of analyses, protein with N-glucosamine groups has more temperature dependence structure. By increasing temperature, the deglycosylation formed a thermostable folding. Thus, glycosylation not only implies its impact on localized residues near the glycosylated sites necessarily, but also propagated to other regions of the protein and increase residues fluctuations and consequently the proteins' radius of gyration (Fig. 1). Root mean square displacement (RMSD) analysis also confirm radius of gyration results, too. We also computed number hydrogen bond, and their lifetimes in mutated and glycosylated forms of Lip2 lipase. These results indicate that by increasing temperature, the non-glycosylated protein folding and number of H-bonds increased. In this regard, the enzyme overall stability decreases rather than the WT with an anonymous molecular mechanism. Due to in silico research into thermo-stability of this protein in aqueous solution, more information about the efficacy of each compartment is provides. As the missing chain, independent presence of glucosamine group is going to be analyzed to recognize the problematic factors.

کلمات کلیدی:

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