The K461Q mutation increases the thermo-stability of β-xylosidase: an in silico study

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Abstract: Xylan is the second (after cellulose) most abundant structural heterogeneous polysaccharide found in plant biomass. Bioconversion of Xylan into fermentable sugars requires its enzymatic hydrolysis into monomeric components [1]. β-xylosidase or xylan 1,4-β xylosidase (EC 3.2.1.37) is considered to be key enzyme in Xylan hydrolysis. This enzyme removes successive D-xylose residues from the non-reducing ends of xylo-oligosaccharides. Due to its significance in industrial Xylan hydrolysis, evolving more thermostable β-xylosidase has contemporary garnered a lot of attention [2]. In the present study, we have launched an in silico study to design a more thermostable β-xylosidase. In this regard, the 3D structure of β-xylosidase (under the PDB ID of 3C2U) was assessed for the thermal-factor values of its amino acids using Chimera software. The Glycine amino acids and the amino acids with highest thermal-factors were chose to be mutated using Molegro software. The Glycine residues were mutated to Proline, while the other amino acids were fed to Rosetta Design software to find amenable mutations. iRDP, Foldx, Imutant and Duet software were used to assess the effects of introduced mutation on the protein stability. Ultimately, the evolutional conservation of the selected mutation was assessed using BLAST search and sequence alignment in NCBI database. The results of performed mutations indicated that the Glycine to Proline mutations failed to enhance the stability. However, the Lysine to Glutamine mutation at position 461 resulted in a more stable enzyme. This mutation have also been shown to be evolutionary favorable. In conclusion, our results indicated that the K461Q mutation harbors the potential to engineer the β-xylosidase to have higher stability and therefore more industrial sufficiency. It seems that using in silico approaches would circumvent the costly and arduous processes of empirical methods and pave the way for future protein engineering studies.

Key words: β-xylosidase; mutation; thermos-stability; in silico analyse

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