STRUCTURAL AND DOCKING ANALYSIS OF A SPIRULINA PLATENSIS DPP-IV INHIBITORY PEPTIDE

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Diabetes is a very common chronic disease defined by high blood glucose levels [1]. Dipeptidyl peptidase IV (DPP-IV) enzyme causes the degredation of glucose-dependent insulin releasing polypeptide (GIP) and glucagon like peptide-1 (GLP1) molecules and consequently the glucose level in the blood is not lowered. Inhibition of DPP-IV enzyme provides an antidiabetic effect by lowering the blood glucose levels [2]. Anti-diabetic drugs have some side effects and limitations, hence research on novel pharmacological molecules has accelerated[2]. Many studies have shown that natural-derived DPP-IV inhibitor peptides have therapeutic potential [3]. Spirulina platensis microalgae was shown to produce a DPP-IV inhibitory peptide identified as LRSELAAWSR [4], but its mechanism of action at molecular level is unknown yet. In this study, the interaction of the peptide with the DPP-IV enzyme was investigated. PEP-FOLD 3.5 was used for peptide structure prediction[5]. The DPP-IV enzyme complex structure was obtained from the PDB (1WCY) and the water and inhibitor molecule were removed before docking analysis. Possible active site amino acids of the enzyme was found in the literature[6]. The interaction was simulated with the HADDOCK docking tool [7] and score of best model was calculated as negative (-70.8 +/- 5.6). The amino acids involved in the interaction were predicted as R560, R358, I407, E408, R356. The DPP IV inhibition mechanism of the Spirulina peptide was modeled as a result of this research. The results of this research will guide our further recombinant peptide production and mutation studies.

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