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Effect of charge change on the EF-hand II recovery in Mnemiopsin 2 by H95D mutation

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Abstract

Bioluminescence is the phenomenon of visible light emission by living organisms which chemical energy is converted into light energy. This globular photoprotein consists of 207 amino acids with a molecular weight of 24 KD. This photoproteins has 4 EF-hand with a helix-loop-helix structure that are Ca^{2+} binding sites. 3 residues, aspartic acid, at position 1; glycine, at position 6, and glutamic acid, at position 12, are conserved. It is worth mentioning that EF-hand II has lost this ability. Also, Mn2 has a hydrophobic cavity that forms coelenterazine binding site. The aim of this work is to investigate the structural and functional properties of the mutated protein H95D in order to recovery the EF-hand II activity. Thus, at first Mnemiopsin 2 amino acid sequence was obtained from the NCBI database and mutant models were designed. Finally, the sequence alignment of the wild-type protein along with the mutant protein, aequorin, obelin, and berovin was aligned with Clustal W and checked by through the ESPript3 server. Using Modeller version 9.20, three-dimensional structures of both wild-type and mutated protein were generated. Using VADAR, SAVES and ModEval servers, the best model was confirmed based on the parameters such as WHATCHECK, PROCHECK, z-DOP, ERRAT and RMSD. The ProtScale server was used to drawing hydropathy plots, while several biochemical parameters were calculated by using ProtParam. The results show that this mutation caused increased the structural stability of the protein.

Key words: EF-Hand, Molecular modeling, Photoprotein, Site-directed mutation

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