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Investigation of Glycin 96 roles in EF-handll photoprotein Mnemiopsin 2: bioinformatics Studies

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Abstract

Bioluminescence is the process of light emission by some living organisms. Mnemiopsin 2, a Ca2+ regulated photoprotein isolated from *Mnemiopsis leidyi*, having a blue flash type emission and belongs to family of ctenophore photoproteins. Photoprotein mnemiopsin 2 is a single subunit protein consisting of 207 amino acid residues. These photoproteins have been exploited as markers or reporters for biochemical processes in biological and biomedical researches. They are precharged bioluminescent proteins that are triggered to emit light by binding Ca^{2+} or certain other inorganic ions. They contain three EF-hand domains to bind Ca²⁺, and accommodate a peroxidized coelenterazine in the central cavity of the protein. Ctenophore photoproteins also contain three canonical sequence loop regions, each of 12 contiguous residues, which supply the oxygen ligands needed for calcium ion coordination. The residue of Glycin 96 is the twelfth residue in the EF-hand II loop of mnemiopsin 2, EF-hand II has lost its function during evolutionary stages. For this purpose, Glycin 96 was replaced with Glutamate residue (G96E). The three-dimensional structure of mutant was made with MODELLER program V. 10.4 and the best structure was evaluated using ModEval, SAVES. VADAR and ProtParam servers were used to calculate the interactions, Structural stability and physicochemical properties of protein. ProtScale server showed Kyte & Doolittle hydropathy plot. Then, the graphical form of the desirable model was drawn using the UCSF Chimera software Finally, the optimized models were compared with the native model. The results indicate that the mutated model is slightly unstable than the native model, And it also increases the polarity in its structure. However, the free energy of G96E mutant has increased compared to native, and indicates the sturactural stability of the mutant.

Keywords: Molecular Modeling, Photoprotein, Site-directed mutagenesis, Stability.





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