

3D modeling of the opsin structure for the gastropod mollusc *Lissachatina fulica* using AlphaFold 2

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Motivation and Aim: The study of protein structure and function is fundamental to understanding life processes at the molecular level. In particular, visual pigments, such as opsins, play a key role in the mechanisms of vision in animals [1]. Obtaining accurate models of the spatial structure of opsins makes it possible to reveal the specific features of their functioning. Current knowledge of these proteins' structure has been obtained mainly in studies on vertebrates, arthropods, and cephalopod molluscs. However, there is little data on the structure of visual opsins in gastropod mollusc and none for terrestrial species. Thus, the aim of this work was to model the 3D structure and determine the most likely candidate for the role of the optic opsin in *Lissachatina fulica*.

Methods and Algorithms: In this work, 5 previously predicted *L. fulica* opsins, Afu011750, Afu004575, Afu005002, Afu003765 and Afu022267, were analyzed. The primary sequences of *L. fulica* proteins were taken from Guo's article [2]. AlphaFold 2 algorithm was used to predict 3D structures [3], visualization and analysis of structural homology of the obtained structures with the 3D structure of rhodopsin *Todarodes pacificus* (RCSB Protein Data Bank database) resolved by X-ray structural analysis with an accuracy of 3.70 Å were performed using PyMol. The structural homology analysis took into account the root mean square deviation (RMSD), which measures how much a particular molecular structure deviates from the reference geometry [4].

Results: By analyzing the structural homology and RMSD obtained by comparing the predicted *L. fulica* opsins with *T. pacificus* rhodopsin, the three sequences Afu005002 (RMSD = 0.916 Å), Afu004575 (RMSD = 1.158 Å), and Afu016848 (RMSD = 2.829 Å) were shown to have the lowest RMSD values and thus the highest structural homology. The influence of the nearest amino acid residues on the positions of the main absorption maximum for Afu005002 was also analyzed. As a result, it was found that the greatest contribution to the absorption spectrum and to the spectral shift of the predicted opsin structure of Afu005002 was made by protonation of Glu175.

Conclusion: Thus, we can conclude that Afu005002 is the most likely candidate for the role of a visual opsin in *L. fulica*. Our study opens new opportunities for further research on opsin proteins, including the study of their visual mechanisms.

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