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Ser 81 of *Natronomonas pharaonis* halorhodopsin plays a role of holding chloride ions near the Schiff base

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In this study, we aim for advanced visual restoration of enhanced contrast by light-driven halorhodopsin into retinal photoreceptor cells and hyperpolarization of optic nerve by light absorption. However, strong light is necessary for the light driving, because halorhodopsin has low photoresponsiveness. Therefore, it is necessary to develop a functionally enhanced halorhodopsin for visual restoration. As basic research, we analyzed the amino acid residues essential for chloride ion pump of halorhodopsin. *Natronobacterium pharaonis* halorhodopsin (NpHR) is a light-driven chloride ion pump. It is necessary to load chloride ions at the binding site-1 (BS1) of Thr126 near the protonated Schiff base in order to make chloride ions to pass through the cell membrane at light absorption. However, the network of hydrogen bonds near the BS1 is complicatedly intertwined and it is not known well yet how chloride ions are retained at the BS1. In this study, we performed a molecular dynamics simulation for wild type and S81A mutant of NpHR structures, respectively to obtain dynamic information of chloride ion at the BS1. As a result, the Thr126 of the wild type retained binding to the chloride ion by hydrogen bond. While, the S81A mutant was unable for chloride ion to retain the position of the BS1 and then the chloride ion was released from there. We found that the side chain of Thr126, which was fixed by hydroxyl group of the Ser81, rotated other direction. Furthermore, NpHR S81A recombinant cell was actually prepared and then was recorded by the patch clamp. It was confirmed that the NpHR recombinant cell did not occurred hyperpolarization and thus it was found that the NpHR S81A did not transport the chloride ion toward cytoplasmic side.

Recent Publications

- Yuko Ishizuka and Takeshi Kikuchi (2011) Analysis of the local sequences of folding sites in beta sandwich proteins with inter-residue average distance statistics. *The Open Bioinformatics Journal* 5:59-68.

Biography

Yuko Sakajiri has her expertise in bioinformatics of protein structure prediction and has passion in visual restore. In a previous study, she studied the protein folding prediction of the beta barrel protein and found several folding patterns in the early stages of protein folding using the average distance map technique. Then, she started the study for visual restore and has predicted the structure of the rhodopsin-like protein and the ion pathway inside the protein. These studies are expected to lead to the development of modified rhodopsin for the improvement of visual restore.

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