

## Distances among Retinal Atoms and Rhodopsin Atoms in Squid Optical Receptor

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At the first, historical speaking was taken that this theme for squid rhodopsin was brought by M. Kito on his interesting about squid sense. Thus M. Kito proposed to investigate the pigments on squid light sense. Our works was started from his interesting. T. Maddess has the interesting on the sense organ on light, and he is an expert on light-sense receptor or pigment. Y. Nagai has many experiences on computer calculations. On these backgrounds of us, we started to investigate squid rhodopsin. Fortunately, four kinds of data for squid rhodopsins are obtained by using the key word “squid rhodopsin” at the protein data bank (PDB). In 2010 we got two kinds of squid rhodopsin data at PDB, and then next year (2011) we got furthermore two PDB data. Then we have four PDB data of squid rhodopsin. We started molecular orbital calculations by the collaboration with H. Kagawa, and we wrote a first paper about the investigations for HOMO and LUMO analysis of squid retina [1]. We show the references [1] and [2] that we done since the repetition is avoided. Retinal structures are shown below. PDB identification codes are 2Z73 and 3AMY for chain A and B. As seen the figure of the conformation for retinal of 2Z73, the structure found in chain A is quite similar to that found in chain B. These two figures for retinal are important to consider retinal contacts with atoms of amino acid residues in squid rhodopsin.

The structure for PDB id 3AYN has turn of straight line that similar to the structure of retinal shown in Fig. 1. As known from Fig. 2, PDB id 3AYM has curved structure about the line ( $C_1$  to  $C_{15}$ ). It is difficult that the conformation is cis-form or trans-form. We guess from the distance between each retinal carbon and atom of amino acid residues of squid rhodopsin. We guess the nearest distance means atomic contact. We evaluate that PDB id 3AYM has the trans-form for retinal. We can recognize that the structure change of direction of retinal ring has occurred on chain A and B of squid rhodopsin.

It is also important what structure rhodopsin has. This fact can be understood to draw contact

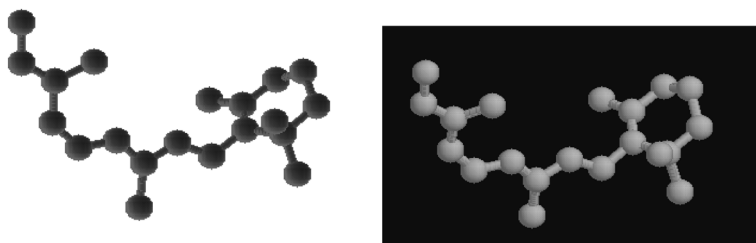


Fig. 1 The left is the retinal found at chain A of 2Z73 and right is that of chain B of 2Z73

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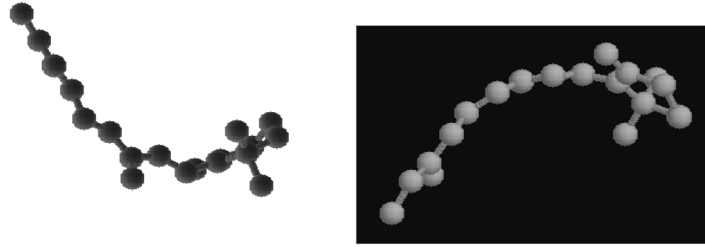


Fig. 2 The left is the retinal structure found at chain A of 3AYM and right is that of chain B of 3AYM.

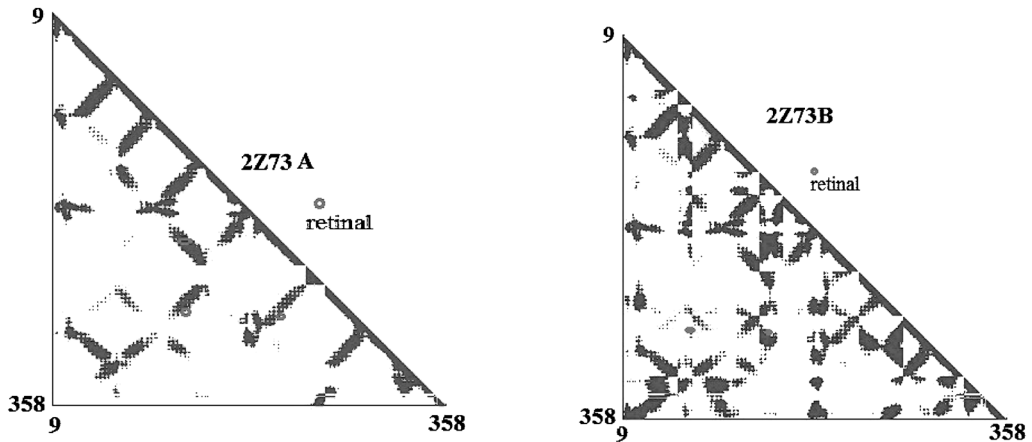


Fig. 3 Retinal location is denoted by circle of weak color on the contact map of rhodopsin. Left side figure denotes contact map of chain A of 2Z73 (2Z73A) with retinal contact estimation for the circle of weak color, and right side figure is contact map of chain B of 2Z73 (2Z73B) with retinal contact (shown by the circles of weak color).

map of rhodopsin. If alpha-carbons make the helix structure, contact is the line parallel to diagonal line. If alpha-carbons take untiparallel beta-sheet, the contact is the line orthogonal to the diagonal line. These things are to understand the contact map. We show the contact map of chain A and B of squid rhodopsin 2Z73 (PDB id) at Fig. 3. Left side figure is given for chain A and right side figure for chain B in Fig. 3..

We also show the contact of retinal carbons with amino acids of squid rhodopsin by the circles of weak color (it is difficult to see). As seen from reference [2], the contact of retinal carbons has sveral sites of contact map. The contact means the nearest distance between each retinal carbon and atom of amino acids of squid rhodopsin, namely they represented as the table of reference [2]. The circles of weak color shown above (Fig. 3) are investigations at this time so that one couldn't found in references [1, 2].

We talked about other found facts, but anyone can understand by reading references [1, 2]. Thus we omitted details that we talked on the speech of memorial workshop of Kazuhide Mori on computatinal sciences for the first time concerning to squid retina and rhodopsin. We summarized new things about retinal and rhodopsin of squid PDB data. We furthermore develop the evidences about squid rhodopsin. The talk was showing found things about squid rhodopsin.

### References

- [1] Y. Nagai, K. Kito, H. Kagawa, T. Maddess, A quantum chemistry of retinal of squid rhodopsin, *Mem. Kokushikan U Cent. Inf. Sci.* **32** (2011) 20–31.
- [2] Y. Nagai, K. Kito, T. Maddess, Spacing between retinal and amino acid residues in squid rhodopsin, *Mem. Kokushikan U Cent. Inf. Sci.* **33** (2012) 1–7.