Dihedral freedom of the chromophore in Channelrhodopsin-modelling its photoisomerism

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Abstract:

Channelrhodopsin is a light gated cation channel that was first discovered in 2002 when the phototaxis of an alga, *Chlamydomonas reinhardtii*, was studied. Channelrhodopsin consists of 737 amino acids, seven transmembrane domains (opsin) and a chromophore (retinal) in the center (Fig 1). The chromophore is an all-trans retinal and is covalently bonded to Lys 296 on transmembrane domain 7. When blue light shines upon the chromophore, the all-trans retinal isomerizes to 13-cis retinal. This induces further conformational changes in the protein resulting in the formation of a pore that is at least 6 Å wide which leads to flowing of cations inside the cell. Because of the similarity of this mechanism to what happens in the firing of action potentials in our nervous system, scientists have utilized this protein to develop a novel technique called optogenetics, which has allowed scientists to activate neurons using light. In this study, we are carrying out computer simulation of the trajectory of channelrhodopsin in its ground state and with freely rotating dihedral in the chromophore around the double bond indicated (by an arrow) in figure 2. The changes in dihedral angles with respect to time in both cases will be studied along with the interaction of the chromophore with surrounding amino acids. This will hopefully reveal useful information about the dihedral freedom of the chromophore in channelrhodopsin during its photoisomerism.

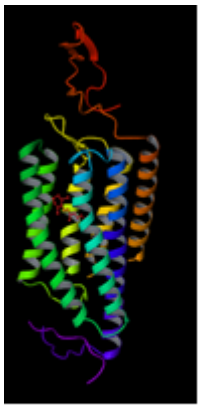

Fig 1
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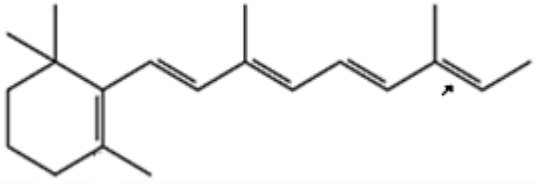

Fig 2