REGULATION OF THE SPECTRAL ABSORPTION OF 11-CIS RETINAL CHROMOPHORE IN RHODOPSIN BINDING POCKET.

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The purpose was to analyze the mechanism regulating the absorbance of 11-cis retinal chromophore bound to specific residue Lys-296 and linked covalently via protonated Schiff base, PSB, positively charged and stabilized by the carboxylic acid residue Glu-113 that serves as the counterion in the visual pigment called Rhodopsin; this aim would help to the understanding of the chemistry and physiology of the vision. The Rhodopsin is a G protein-coupled receptor, specialized for detecting photons and essential in the photoreceptors for scotopic and peripheral vision in humans; its maximum peak of absorption is close to 500 nm. The chromophore for others visual pigments absorbing at 425, 530 and 560 nm, is equal and linked for the same PSB.

However, the opsin protein is different, this points to a decisive effect of proteic environment on the spectral tuning. For calculations was used a SCC-DFTBoptimized model for the binding pocket of Rhodopsin, which is based on chain B of crystal structure of Rhodopsin with 2,2-Å of resolution (1U19) and taken from a previous study, in order to evaluate the effect of aminoacid residues located inside a sphere of 6-Å around the chromophore on spectrum of absorption. The spectrum of absorption was calculated with NDOL, a quantum chemical method, *a priori,* allowing the calculations with complete geometry of analyzed system; important contributions to the spectrum of absorption were found for counterion Glu-113 and others residues of the binding pocket of Rhodopsin.