THEORETICAL CALCULATIONS OF THE ENERGY BALANCE OF TWISTING ATP SYNTHASE b_2 SUBUNITS

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The process of oxidative phosphorylation in mitochondria and bacteria, or photophosphorylation in chloroplasts, requires the enzyme F1Fo-ATP synthase to utilize the energy of the transmembrane proton gradient for the production of ATP from ADP and Pi. The structure of ATP synthase is traditionally divided into the water soluble F1 domain, comprising subunits α3, β3, γ, ε and δ, and the membrane bound Fo domain harboring the proton transporting c-ring and a, b2 subunits. It is known that the dimerization domain of b subunits contains a two-stranded right-handed coiled coil with offset helices. However, the role of the homodimeric b2 subunits is still unclear. We propose a mechano-chemiosmotic mechanism [1] of ATP synthesis. According to this model the coiled-coil b2 subunits are the ropes that are shortened by binding of phosphate ions to positively charged lysines or arginines, which results to pulling of α3β3-hexamer to the membrane during energization. In order to evaluate the energy efficiency of such twisting we calculated the energy balance in binding phosphate ions to protonated residues of arginine and lysine. The energy of binding equal to -0.69 kcal / mol in the base state and 8.14 kcal / mol after phosphatization of the protonated groups at a value equal to the dielectric constant of 15.57. Negative energy figure shows the stability of the system, and a positive value on the implementation of the positive work in which energy is decreasing waning. Our calculations show a hyperbolic dependence of the interaction energy on the dielectric constant. Obviously, the dielectric constant in this case, indicates the amount of water in the matrix. These data are very useful for understanding the mechanism of aging, since during the aging decreases the amount of water in the cell as compared to a young body and an old body is experiencing a lack of energy.

References

1. *Kasumov EA, Kasumov RE, Kasumova IV.* A mechano-chemiosmotic model for the coupling of electron and proton transfer to ATP synthesis in energy-transforming membranes: a personal perspective //*Photosynthesis Research*, **Vol. 123**, 2015. Pp. 1-22.