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Electrostatic spacing dependent conformation of a pair of α-helices of Voltage-gated K+ ion channel

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Abstract : Voltage-gated K+ ion channels of Aeropyrum pernix(KvAP), a trans-membrane protein controls the flow of potassium ions in response to voltage-gradient. This tetramer protein consists of Voltage Sensor Domain (VSD) which senses the voltage and Pore Domain(PD) which guides the ions through the pore. Each monomer comprises of three antiparallel pair of α-helices, which behave like a macrodipole with positive N-terminal and negative C-terminal charges on either end of the helices. Such four (S1-S2, S3-S4) macrodipole α-helices are in VSD and two (S5-S6) in PD. As S3 helix has two segments, S3a and S3b, there are several experimental evidences, including X-Ray crystallography showing S3b-S4 pair as a single unit, but their mutual conformation at different voltage is still unknown. Our group has theoretically shown that at zero voltage the strong electrostatic attraction between S3b-S4 has kept them inseparable and the conformation obtained is very similar to the pdb structure by computing the system with two degrees of freedom (one translational and one rotational). Here we have tried to show a refined conformation of the α-helix pair with six degrees of freedom (three translational and three rotational) for each macrodipole. Using our innovative software, the change in the conformation of the 3-D structure of S3b-S4 α-helix pair of VSD with various separations between two helices is studied. Statistical data obtained indicates that, with different electrostatic spacing: (1) the stable minimum potential energy differs; (2) the stable conformation of the S3b-S4 α-helix pair changes.

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