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Conformational stability of α-helices of VSD of K+ ion channel in hybrid dielectric media of neuron environment

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Abstract Ion-channels, involved in transmission of nerve impulses, undergo reversible conformational changes under the influence of electrical field. The voltage-gated K^+ ion-channel of *Aeropyrum pernix*(KvAP) is an aggregate of α-helical protein with two domains: the voltage sensor domain(VSD) responds to the varying trans-membrane voltage gradient controlling the flow of ions and pore domain(PD) allows the passage of K^+ ions across the bilayer membrane. Each α-helix, behaves like a macrodipole with two inherently equal and opposite poles (+N-terminal and -C-terminal) of half-electronic charges, apart from the polar, non-polar and charged residues, which interact with lipid bilayer and cellular ionic solution, forming a specific hybrid dielectric environment. X-ray and solution structures of KvAP [Jiang 2003a, Mackinnon 2010] show that all the alpha-helices (S1-S2, S3-S4, S5-S6) in full length KvAP are not only pair wise mutually anti-parallel but spatially they are not identical in orientation. Our electrostatic theory shows that at zero voltage their anti-parallelism minimizes the potential energy for stability and the variation of exposure of the terminal charges and the charged residues to different media alters the conformation of the system. The relative angular orientation of S3b-S4 macrodipole pair and their separation gives their mutual configuration which varies with exposure to hybrid dielectric media as all charges try to accommodate in their optimum environment so that the whole system gets energetically minimized.