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Homology Modeling and Molecular Dynamics Simulation Study for TREK-2 Potassium Channel

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Potassium (K^+) channels are found in the plasma membrane of virtually all types of cells and perform important cellular functions such as regulation of cell excitability, cell volume, cell growth and proliferation, and even cell death. K^+ channels share a common selectivity filter that determines the conduction characteristics of the pore. All K^+ channels contain a highly conserved sequence, the P domain, which forms the selectivity filter. The two-potassium channels (K2P) are found widely, from single-cell yeast to plants to higher mammals. K2P channels are key role in the cellular mechanisms of neuroprotection, anaesthesia, pain and depression and modulated by cellular lipids and pharmacological agents, polyunsaturated fatty acids, volatile general anaesthetics. These channels contain four transmembrane segments (4TM) and two pore-forming domains (2P). TWIK-related K^+ channel-2 (TREK-2), is one of the K2P channels, a new member of the mechanosensitive tandem-pore K^+ channel family, share 65% amino acid sequence identity with TREK-1. This channels expressed in both CNS (Central Nervous System) peripheral tissues and also DRG (Dorsal Root Ganglion). It is involved in amount of pathologic process such as acute cerebral ischemia and associate with nociception and tissue distribution. In order to understand mechanism of TREK-2 protein, molecular dynamics (MD) simulations were performed with lipid bilayer and water systems. First homology model of TREK-2 was generated by *MODELLER* in Discovery Studio 2.0 using NaK channel (PDB ID: 2AHZ) as template. And MD results will be discussed.