



سمینار هفتگی گروه ماده چگال نرم

Simulation of interaction between a small scorpion toxin with potassium channel

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Toxic peptides have a significant role in understanding structural behavior of potassium channel. The interaction of a small peptide purified and identified from an Iranian scorpion venom, BmPo2, with potassium ion channel, rSK2, was simulated by successive application of Brownian and molecular dynamics simulations. Our simulations revealed two lysine residues of BmP02 located in loop connecting the alpha-helix and beta-sheet contribute in complex formation. We think this is a new mode of interaction in which the toxin vertically oriented on top of channel and this can provide an explanation for weak toxicity of BmP02.

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