

Abstract

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Project Title : Study of selectivity ion conduction in Na⁺ channel by Statistical integral equation theory

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Abstract:

Selectively transport of Na⁺ and K⁺ across cells provides the electrical signal in cardiac, muscle and nerve cells. To understand the basis of discrimination between Na⁺ and K⁺ of sodium channel, we investigate the ions distributions in the selectivity filter of voltage gate sodium channel by applying the 3D-RISM theory. The distribution function of water and ions, Na⁺, K⁺ and Cl⁻, in the channel were calculated. Our results show the ion binding at S1, S2 and S4. The PMFs from the implicit ion model show the highest ion selectivity arises at the S2 site. The explicit ion model demonstrated the selectivity arise because the difference of dehydration water molecule between Na⁺ and K⁺.

Keywords : 3-5 words

Sodium channel, ion channel, 3D-RISM, selectivity