Monte Carlo Simulation for Statistical Mechanics Model of Ion Channel Cooperativity in Cell Membranes

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Abstract

Voltage-gated ion channels are key molecules for the generation and propagation of electrical signals in excitable cell membranes. The voltage-dependent switching of these channels between conducting and nonconducting states is a major factor in controlling the transmembrane voltage. A statistical mechanics model of these molecules has been discussed on the basis of a two-dimensional lattice model in a square lattice with nearest neighbour cooperative interactions. A new Hamiltonian and a new Monte Carlo simulation algorithm are introduced to simulate such a model. Sigmoidal-shaped curves are found for the fraction of channels in open state at equilibrium (\(p_o\)). When there is no interaction between channels the theoretical model well matches the experimental data obtained from batrachotoxin-modified sodium channels in the squid giant axon using the cut-open axon technique. Cooperative interactions alter the position and shape of the curves and change the slope at the midpoint of \(p_o\) versus voltage curve.