Computing Characterizations of Drugs for Ion Channels and Receptors Using Markov Models (Lecture Notes in Computational Science and Engineering)

Aslak Tveito, Glenn T. Lines

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Flow of ions through voltage gated channels can be represented theoretically using stochastic differential equations where the gating mechanism is represented by a Markov model. The flow through a channel can be manipulated using various drugs, and the effect of a given drug can be reflected by changing the Markov model. These lecture notes provide an accessible introduction to the mathematical methods needed to deal with these models. They emphasize the use of numerical methods and provide sufficient details for the reader to implement the models and thereby study the effect of various drugs. Examples in the text include stochastic calcium release from internal storage systems in cells, as well as stochastic models of the transmembrane potential. Well known Markov models are studied and a systematic approach to including the effect of mutations is presented. Lastly, the book shows how to derive the optimal properties of a theoretical model of a drug for a given mutation defined in terms of a Markov model.

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