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Investigation of the kinesin stepping mechanism via simulated annealing[1] B.D. JACOBSON, S.J. KOCH, S.R. ATLAS, Department of Physics and Astronomy, University of New Mexico — As kinesin processes along the microtubule, the cycle of different chemical states and physical conformations that the protein assumes can be represented by a kinetic model. Such models are preferred for numerical calculations since information about the kinesin stepping mechanism at all levels, from the atomic to the microscopic scale, is fully contained in the particular states of the cycle, in how states transition, and in the rate constants associated to each transition. This greatly simplifies the model of the mechanism while providing a reliable physical picture. We have developed a methodology that optimizes a kinetic model for kinesin built with a minimum of a priori assumptions about the mechanism. We combine Markov chain calculations and simulated annealing optimization to find the rate constants that effectively fit experimental data on kinesin speed and processivity. This optimization scheme leads us to choose the cycle that is most likely to realize the kinesin step. We report details of our kinetic model simulations which best fit experimental data for both single-molecule and gliding motility assays at varying ATP concentrations.

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