

Mathematical Modelling of Protein Structure and Function

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Abstract

In this talk I will briefly describe the mathematical techniques used to model the protein structure. This will be illustrated with several key examples of functional proteins such as actin, kinesin and tubulin. The structure determination calculations will then be used to predict the behaviour of protein aggregates. Consequently, we will see the emergence of polymerization for actin and tubulin. The introduction of motor proteins to solutions containing filaments will result in a qualitatively new behaviour, i.e processive motion of motors. A short discussion will be given regarding the types of mathematical models currently in use for motor proteins. We will critically review the application of Langevin equations, Fokker-Planck equations and chemical kinetics formalism. Finally, we propose a new model of the two-headed kinesin's walk along a microtubule treating its heads as extended objects that are connected by an elastic neck linker region. In our simple mathematical model, ATP hydrolysis provides the chemical energy and directed binding plays the key role in force generation coupled with the presence of elastic neck linker region that stores mechanical energy. The electrostatic charge distributions known for both the kinesin motor domains and tubulin are also shown to be consistent with the physical picture presented here. Our computer simulations based on the model developed here are in good agreement with experimental observations not only for kinesin but also for its analog Ncd. Joint work with H. Bolterauer (J. Liebig University).