MASTER'S THESIS

A computational study of energy conversion efficiency of F1-ATPase

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ABSTRACT

ATP synthase (F_1F_O-ATPase) is an essential enzyme for life. Powered by an electrochemical proton gradient, it catalyzes ADP and phosphate into ATP. The F_1-subunit of ATP synthase is called F_1-ATPase as it also independently catalyzes the reverse reaction in absence of F_O-part. The nearly 100% energy conversion efficiency of the molecular motor has attracted the attention of many physicists and biologists to explore the underlying thermodynamics. Recently, a new nonequilibrium equality derived by Harada and Sasa (Harada & Sasa, 2005) was applied to the experimental time series data on F_1 -ATPase to extract heat flow to the environment. A phenomenological model for rotary motion was proposed and shown to reproduce key experimental features. Interested in the high efficiency of F_1-ATPase and the good performance of the corresponding model, we carried out a detailed computational study of the model to understand its behavior in a broader range of parameter values. We solved the model using a modified Gillespie algorithm for stochastic simulation and by integrating the Fokker-Planck equation. Various physical properties of the model, such as the relation between rotational velocity and parameters characterizing angular dependence (q) and ATP switching rates (W), the relation between two kinds of dissipation and rotational velocity, the negative heat flow from environment to system through ATP binding etc. are analyzed in detail. Importantly, we modified the driving potential to investigate the factors affecting the efficiency. Additionally, we found some inconsistences between properties of this model and previous studies and we could unify them by some adjustments, which may be useful for constructing more precise models in the future.

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