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Tail-Binding Effect of Kinesin-1 Auto Inhibition Using Elastic Network Model

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Abstract : Kinesin-1 (hereafter called kinesin) is a molecular motor protein that moves cargos toward the end of microtubules using the energy of adenosine triphosphate (ATP) hydrolysis. When kinesin is inactive, its tail autoinhibits the motor chain in order to prevent from reacting with the ATP by cross-linking of the tail domain to the motor domains at two positions. However, the morphological study of kinesin during autoinhibition is yet remained obscured. In this study, we report the effect of the binding site of the tail domain using the normal mode analysis of the elastic network model on kinesin in the tail-free form and tail-bind form. Considering the relationship between the connectivity of conventional network model with respect to the cutoff length and the functionality of the binding site of the tail, we revaluated the network model to observe the key role of the tail domain in its structural aspect. Contingent on the existence of the tail domain, the results suggest the morphological stability of the motor domain. Furthermore, employing the results from normal mode analysis, we have determined the strain energy of the neck linker, an essential portion of the motor domain for ATP hydrolysis. The results of the neck linker also converge to the same indication, i.e. the morphological analysis of the motor domain.

Keywords : elastic network model, Kinesin-1, autoinhibition
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