Unveiling Molecular Mechanisms of Kinesin-5

Aram Davtyan¹, Qian Wang², and Anatoly B. Kolomeisky³

Short Abstract — Molecular motor protein Kinesin-5 (Eg5) is a member of kinesin superfamily that is critical for bipolar spindle assembly and spindle maintenance during mitosis. As a result it is a promising chemotherapeutic target for cancer treatment. While a number of small-molecule drugs that interact with Eg5 have been identified, little is known about the molecular mechanisms by which they inhibit Eg5 function. Furthermore, multi-motor systems can exhibit qualitatively diverse behavior for different drugs, in some cases showing non-linear dependence of motor velocity on

drug concentration. We study molecular mechanisms behind function of individual Eg5 and multi-motor systems involving it using computational modeling techniques. Besides apparent fundamental value this work has direct implications for clinical applications, where in depth understanding of Eg5-drug interaction is important.

Keywords — Motor proteins, Kinesin-5, computational modeling.

²Center for Theoretical Biological Physics, Rice University, Houston, TX. E-mail: <u>qw9@rice.edu</u>

³Center for Theoretical Biological Physics, Department of Chemistry, Department of Chemical and Biomolecular Engineering, Rice University, Houston, TX. E-mail: tolya@rice.edu