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Structure-based simulations of kinesin motor domain for the study and characterization of its different microtubule and ligand-binding states SRIRUPA CHAKRABORTY, WENJUN ZHENG, State University of New York at Buffalo — Kinesins are molecular motors acting as enzyme-based nanomachines that transport intracellular cargo along microtubules (MT). To obtain a detailed structural and energetic picture of the various conformations of the kinesin motor domain, we built atomistic models using available crystal structures, homology modeling and flexible fitting into cryo-electron microscopy (EM) maps. These models depict the various biochemical states of the kinesin head, such as - with the neck-linker docked and undocked in the MT-free state, and the different nucleotide (ADP, ATP and APO) bound states in the kinesin-MT complex. Here we perform molecular dynamics simulation techniques and large-scale computational probing of differences in these states, by an exhaustive search of interactions that differ between them, identify key residues in the active site and binding interface, and investigate the binding free-energy between kinesin and MT, and kinesin and ligand to compare with experimentally obtained results.

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