Essential dynamics of tubulin in a microtubular fragment

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Microtubules are dynamical cell structures experiencing complex rearrangements during their growth and shrinkage [1]. Microtubular dynamics is associated with conformational changes in tubulin, which is a building block of the microtubule [2]. Naturally, tubulin interacts with multiple molecules and proteins. Motions responsible for protein functions are forming an essential conformational space. An analysis of such space helps to assign principal motions to functional properties, e.g mechanism of actions of anti-cancer drugs targeting tubulin [3].

In this work we employ the all-atom molecular dynamics simulations to follow the principle motions of tubulin molecules in a wall of the microtubule. Modelling system was prepared based on a minimal fragment of the microtubule. Simulations allow to follow and differentiate principle modes of individual tubulin units depending on their position in the microtubule, which in turn gives an insight into dynamics of both ends of the microtubule in particular.

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