ACTIN MONOMER-MONOMER INTERACTION – A MOLECULAR MECHANICS STUDY

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Abstract

Knowledge of the interaction properties of the actin monomers is critical for understanding the molecular mechanism of the filament polymerization. The aim of the present paper was to provide information about the interaction properties of actin monomers using molecular mechanics approach. In order to be characterized, the atomic structure of the protein was taken from the Protein Data Bank. We used the atomic coordinates set in 1ATN.pdb which is a 3D-model of the actin monomer from rabbit. The commercial software package used to perform the molecular simulations was Hyperchem 6.01. Using the molecular mechanics approach, the interaction energies between actin monomers were evaluated for different intermolecular distances, after a preliminary minimization. Starting from these values, the binding force and binding stiffness were calculated as the first and the second order derivative of the interaction energy with respect to the intermolecular distance. According to the results of our simulations results, the complex between the actin monomers is characterized by a minimum interaction energy of -740.6 kJ/mol and a maximum binding force of about 3.2 nN. Our results match a number of experimental data, thus supporting the idea that molecular mechanics may be a powerful tool to find a way to characterize biological macromolecules.

Key words: actin monomer, interaction properties, molecular mechanics

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