Nanochemistry and biotechnology – POSTER PRESENTATION

Computer simulations of homocysteine molecules embedded in high-density lipoprotein

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Excessive level of homocysteine is a factor increasing the risk for cardiovascular diseases and other ailments. In this paper we applied molecular dynamics method to study the homocysteine system embedded into high-density lipoprotein. HDL aggregate removes cholesterol from artery walls. We fill the aggregate with almost 700 biologically important homocysteine molecules.

The calculations were performed in the physiological temperature T = 310 K. HDL container was simulated both with water and without it, to estimate the impact of water on the dynamics of the molecules inside it. Moreover, the behavior of homocysteine molecules in HDL was compared with their dynamics in pure cluster consisted of the same number of homocysteine molecules, which were placed inside the lipoprotein.

The structural and dynamical observables (mean square displacement, diffusion coefficient, second rank order parameter, Lindemann index and radial distribution function) are discussed. We have found that although the dynamics of homocysteine molecules does not strongly depend on the surrounding HDL water presence, the differences in dynamics between molecules in pure cluster and these embedded in HDL are clearly observed.