Nanochemistry and biotechnology – POSTER PRESENTATION

Molecular dynamics simulations of N-acetyl-p-aminophenol molecules embedded in high-density lipoprotein

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N-acetyl-p-aminophenol, well known as paracetamol or acetaminophen, is a widely used as a pain reliever or a fever reducer. In our computer studies we embedded the paracetamol molecules in high-density lipoprotein (HDL). HDL lipoprotein, which exhibits ability to prevent atherosclerosis by removing cholesterol from blood arteries, was filled with the paracetamol molecules. HDL aggregate, prepared that way, can be treated as a nanocontainer for a selective drug delivery to the different parts of human body.

In our studies we put various number (n = 50, 100, 150) of acetaminophen molecules into the HDL lipoprotein. The calculations were performed, in water environment, for four temperatures, including physiological (T = 290, 300, 310 and 320 K).

The structural and dynamical observables of cholesterol (mean square displacement, diffusion coefficient, second rank order parameter, Lindemann index and radial distribution function) are presented and discussed. We have found that HDL adapts its shape to the size of embedded paracetamol cluster.

Our research indicates that paracetamol forms solid phase in the confinement.