Nanochemistry and Nanobiotechnology

Computer simulation of cholesterol molecules embedded in high-density lipoprotein

Z. Gburski[1], M. Pabiszczak[1], P. Raczyński[1]

[1] *Institute of Physics, University of Silesia, Uniwersytecka 4, 40-007 Katowice, Poland.*
E-mail: zgburski@us.edu.pl

Low levels of HDL have been implicated in the increased risk of coronary artery disease [1,2].The dynamics of cholesterol molecules embedded in high-density lipoprotein has been studied using computer simulation technique. The calculations have been performed for the physiological temperature T = 310 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. The corresponding characteristics of pure cholesterol cluster were also calculated. We have found that the dynamics of cholesterol molecules in a free cluster differs from the case of cholesterols embedded inside high-density lipoprotein.

The dynamics of 1-palmitoyl-2-oleoyl-*sn*-glycero-3-phosphocholine (POPC) molecules forming the outer layer of high-density lipoprotein has been studied. We show that it is slightly influenced by the water surrounding lipoprotein aggregate.

1. *Fielding C.J.* High-density lipoproteins: from basic biology to clinical aspects, Wiley-VCH, Weinheim, 2007.
2. *Kontush A., Chapman M.J.* High-density lipoproteins structure, metabolism, function, and therapeutics, John Wiley & Sons, Inc., Hoboken, N.J., 2012.