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C_{60} fullerene interacts with human serum albumin

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The unique properties of C_{60} fullerenes have raised the interest of using them for biomedical applications. Nanomaterials in a biological environment interact with proteins. The most abundant blood plasma protein is a human serum albumin (HSA), which transports fatty acids, hormones and drugs. The aim of this study was computational modeling of the interaction of HSA with C_{60} fullerene and estimation of the size distribution of C_{60} fullerene particles in various physiological media.

By using molecular simulation it was found that C_{60} fullerene can interact with HAS, specifically with following amino acids residues: ASP 451, Ser 342, Lys 190 in the case of the first binding pocket and Arg 428, His 510, Lys 524, Glu 520 in the case of the second binding pocket.

The distribution of C_{60} fullerene particles on the size and number in water solution without chemical dispersants with different salts and HSA was evaluated using the correlation spectroscopy analysis. In particular, it is shown that C_{60} fullerenes in water colloid solution and saline (0,9% NaCl) form both single molecules as well as aggregates with diameter from 38 to 600 nm. HSA introducing into saline promotes dispersed state of C_{60} fullerene particles and prevents their spontaneous as well as NaCl-dependent agglomeration. This directly indicates the prospects of using C_{60} fullerenes for biomedical studies.