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Shape reconstruction of nanoparticles in clusters using SAXS data

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The level of structural information that can be obtained from small angle X-ray scattering (SAXS) data generally is determined by the nature of the scattering objects. For monodisperse systems of identical particles SAXS intensity is directly related to the structure and provides the unique opportunity to determine their shape and size, and in some cases, the internal structure with resolution of about 1 nm. However, in practice, the samples may contain some amount of aggregates or clusters, which cannot be removed from the specimens by conventional methods of purification due to association effects which are essential features and functional properties of some biomacromolecules. Thus, to reveal a structure of individual scattering objects in the associates and to determine their mutual packing within the clusters is of great practical interest. In the present work a large series of computer simulations was made to reconstruct structures of clusters composed of geometrical bodies ("monomers") different in size, shape and mutual arrangement. The task was complicated by certain polydispersity of the associates. *Ab initio* low resolution shape restoration of the "monomers" and of the clusters was performed by a program DAMMIN based on the simulated annealing minimization procedure [1]. Shape of the "monomers" was chosen using information about actual problems arising in structural studies of proteins due to their properties of inherent self-assembly. As a result of the modeling conclusions on the certain limitations and applicability of the shape restoration of macromolecules within clusters were made.

[1] D. I. Svergun, *Biophys. J.* **76** (1999) 2879-2886.

P-03

Interaction of selected gemini surfactants with two model proteins: BSA and HEWL

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The protein-surfactant interactions has been examined over a few past decades, as this problem is vitally important due to its prospective applications of surfactants in medicine, biotechnology, food industry and many others. Proteins bind various substances, giving complexes. The research on protein-surfactant interactions can help to understand the influence of surfactants on processes of denaturation, solubilization and renaturation of proteins. Another fundamental process set under researchers scrutiny is protein aggregation, underlying numerous severe human neurodegenerative diseases and being often considered as undesired effect in biotechnology.

Gemini surfactants is a group of novel and very interesting surfactants. The gemini molecules consist of two polar heads interconnected via a spacer group and bound to two hydrophobic chains. They exhibit very low critical micellization concentrations (cmc), a diversity of forms, making their properties easily adjustable, and they can assemble into micelle-like structures similar to biological membranes.

Bovine serum albumin (BSA) is an important transport protein binding various ligands, including fatty acids and metals. Hen egg white lysozyme (HEWL), on the other hand, is a well-known model protein for studies of aggregation phenomena.

The investigation of interaction of BSA and HEWL with gemini surfactants has been carried out with use of three different techniques: small angle X-ray scattering (SAXS), circular dichroism (CD) and nuclear magnetic resonance diffusiometry (NMRD). Its results will be presented at the conference.

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