

Self-Assembly of Amphiphilic Molecules and Prediction of the Partition Behavior of Different Solutes in the Micelle/Water System

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In this work the self-assembly of different amphiphilic molecules is investigated. Amphiphilic molecules such as surfactants and lipids can be divided into different classes according to their headgroup charge. For this reason different surfactants are chosen as representatives for each class: SDS (anionic), CTAB (cationic), LysoPC (zwitterionic) and Brij35 (nonionic). The self-assembly is simulated by all-atom molecular dynamic (MD) simulation with the Charmm36 forcefield. The probability of different micelle sizes is estimated and compared to experimental data. Beside the size of micelles the shape and stability are very important properties for the characterization of the structures. For ionic surfactants or lipids counterions are taken into consideration. The ion distribution profile at the surface of the micelles is analyzed, as well as its influence on solute molecules, which can enter the micelles. The retrieved structures can afterwards be combined with the model COSMO-RS, which is based on quantum chemical calculations in combination with statistical thermodynamics. The free energy profile of different small solutes can be calculated with the extension of COSMO-RS, named COSMOmic. Thereby the most probable position of a solute within a micelle can be predicted as well as the partition coefficient for the system micelle/water. The results of the predictions are in good agreement with own experimental data. Furthermore, compared to pure MD simulations, the combination of all-atom MD with fast COSMOmic calculations, gives comparable good predictions in a significant shorter simulation time.