Molecular dynamics study of propyl gallate in SDS micelles

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Solublization in micellar surfactant solutions is important as far as biological, pharmaceutical and industrial processes are concerned. For example, in pharmacy micelles are used as containers for drug molecules, in industry solubilization plays a key role in detergency, cosmetics, oil recovery and separation.

To study micellar systems molecular dynamics simulations can be applied. The all-atom (AA) simulation gives detailed insight into surfactant molecules and solubilizate interactions as well as structure of formed aggregates. However, the AA simulations of micellar systems are time-consuming and limited to relatively small length and time scales. To extend time and length scales, force fields based on the concept of coarse-graining are developed. Recently this kind of force field has been developed by Marrink et. al.[1] Their MARTINI force field has been successfully applied to protein, nanoparticle and membrane systems as well to study surfactant systems.

In this work, coarse-grain molecular dynamics simulations were presented for sodium dodecyl sulfate micelle in the presence of small organic compounds which solublize into surfactant micelles.