P.49 Atomistic description of the solubilisation of testosterone propionate in a sodium dodecyl sulfate micelle

D Allen[1], Y Saaka[2], M J Lawrence[2] and C D Lorenz[1]

[1]Theory & Simulation of Condensed Matter Group, Department of Physics, King's College London, UK,
[2]Pharmaceutical Biophysics Group, Institute of Pharmaceutical Science, King's College London, UK

Amphiphilic molecules consist of polar head groups and nonpolar tails. Due to this chemical composition, amphiphilic molecules are known to self-assemble into a variety of aggregate structures in aqueous solutions, including micelles, bilayers, vesicles and lamellae. In all of these aggregate structures, the hydrophobic (nonpolar) parts of the molecules assemble to form an apolar interior of the aggregate, from which water is expelled, and the hydrophilic head groups of the molecules are found at the aggregate/water interface. The hydrophobic microenvironment that results from the aggregates in solution can be used to enhance the aqueous solubility of other slightly soluble nonpolar substances. This phenomenon is called "solubilisation". The solubilisation of molecules plays an important role in a variety of industrial and biological processes (including the design of cleaning agents, cosmetics, & pharmaceuticals). Despite the broad application of micelles for solubilisation, the molecular picture of the solubilisation process is not well understood.

In this presentation, we will report the results of molecular dynamics simulations in which we study the solubilisation of testosterone propionate in sodium dodecyl sulfate (SDS) micelles. SDS is a commonly used amphiphilic molecule in the pharmaceutical formulations, which has a twelve carbon hydrophobic tail and an anionic headgroup. We have conducted molecular dynamics simulations of SDS micelles with and without testosterone propionate in an aqueous solution. We will report on how the presence of the drug molecules in the micelles affects the structure, size and shape of the SDS micelle. As the drug molecules are solubilized by the the SDS micelle we will investigate how the interfacial properties of the SDS micelle alters, and also how the solvation of the drug molecule changes. Finally, we will provide a detailed description of solubilisation process of the testosterone propionate, and in turn provide a description of the atomistic interactions, which govern this process. Where appropriate these results will be compared to and verified with the results from small angle neutron scattering experiments.