

Molecular dynamics simulation of oleyl oleate swollen micelles system.

ABSTRACT

Problems with transdermal drug delivery were directly associated with the skin barrier which is the lipid bilayer at the stratum corneum. Chemical penetration enhancers such as swollen micelles that formed from the solubilisation of the surfactants in the nano-emulsion system could provide an effective solution. However, the structural properties of swollen micelles from nano-emulsions of palm-oil esters, whose behaviour is related to colloidal systems, have not been studied in great detail. In this paper, we report on the use of molecular dynamics (MD) simulations to investigate the structural properties of swollen micelles of oleyl oleate (OE). Five series of 10 ns MD simulations were performed at different micelle compositions to determine the structural evolution of OE/Span20 (S20) swollen micelles. We also carried out four MD simulations on the structure of S20, OE/S20, Tween80 (T80) and OE/T80 micelles to study the effect of different surfactants and the addition of OE into the systems. The shapes of the swollen micelles were observed to vary by the difference in the micelle composition, the surfactants used and the addition of OE. The results were correlated with published theory, and consistent with experimental results on the phase behaviour of the nano-emulsion system.

Keyword: Molecular dynamics; Oleyl oleate; Swollen micelle; Nano-emulsions.