Molecular dynamics simulation of palm-based nano-emulsion system

ABSTRACT

Nano-emulsions of oleyl oleate posses the potential to act as penetration enhancers in pharmaceutical applications. However, information on the phase behavior of oleyl oleate nano-emulsions which obtained through laboratory experiments was insufficient to describe the structural mechanism of the self-assembled system. In this research, the structural and dynamical properties of the palm-based nano-emulsions to act as penetration enhancer were studied by computer simulations. The structural and dynamical information of the nano-emulsions were obtained using molecular dynamics (MD) simulation method. The nano-emulsions system comprised of oleyl oleate (oil) with Span20 and Tween80 as the non-ionic surfactants was simulated in the presence of water molecules (oil-in-water system). The effect of lipid composition in the nano-emulsions system was determined by 5 series of MD simulations up to 2.5 ns. The simulation results showed that different shapes of the nano-emulsions were formed as the composition of oil was increased. The critical micelle concentration was found at 20% ï 30% of lipid composition while the higher concentrations lead to the formation of lamellar system. Larger system with random initial configuration was used to simulate the self-assembly characteristics of the nano-emulsions system. The aggregation and disaggregation of the oil and surfactant molecules were observed throughout the simulation.

Keyword: Molecular dynamics; Palm-based; Nano-emulsion; Micelle; Self-assembly