Computational simulation of palm kernel oil-based esters nano-emulsions aggregation as a potential parenteral drug delivery system

ABSTRACT

The self-assembled structure of palm kernel oil-based esters (PKOEs) nano-emulsions has shown a great potential used for parenteral drug delivery applications. Here, all-atom level molecular dynamics (MD) was applied to investigate the aggregation process of PKOEs nano-emulsion system. The system consisted of palm kernel oil-based esters (PKOEs) and dipalmitoylphosphatidylcholine (DPPC) in water. The ratio of all constituents was taken from the homogenous region of a ternary phase diagram determined experimentally. The molecules started to aggregate very rapidly from random configurations. A doughnut-like toroidal assembled structure formed at 50 ns with PKOEs surrounded by DPPC molecules. The structural and dynamical properties of the self-assembled doughnut-like toroidal aggregate were analyzed using the principle moment of inertia, eccentricity and radius of gyration. The aggregation structures were compact with the average radius of gyration of 4.10 (±0.02) nm over the last 5 ns. Additionally, both hydrophobic and hydrophilic interactions were involved in aggregation process with a total solvent accessible surface area of 551.72 (±5.88) nm2.

Keyword: Palm kernel oil-based esters; Dipalmitoylphosphatidylcholine; Self-assembly; Doughnut-like toroidal; Molecular dynamics simulation