**Self-assembly formation of palm-based esters nano-emulsion: a molecular dynamics study**

ABSTRACT

Palm-oil esters (POEs) are unsaturated and non-ionic esters that can be prepared by enzymatic synthesis from palm oil. Their nano-emulsion properties possess great potential to act as drug carrier for transdermal drug delivery system. A ratio of 75:5:20 (water/POEs/Span20) was chosen from homogenous region in the phase diagram of our previous experimental work to undergo molecular dynamics simulation. A 15 ns molecular dynamics simulation of nano-emulsion system (water/POEs/Span20) was carried out using OPLS-AA force field. The aggregations of the oil and surfactant molecules are observed throughout the simulation. After 8 ns of simulation, the molecules start to aggregate to form one spherical micelle where the POEs molecules are surrounded by the non-ionic surfactant (Span20) molecules with an average size of 4.2 ± 0.05 nm. The size of the micelle and the ability of palm-based nano-emulsion to self-assemble suggest that this nano-emulsion can potentially use in transdermal drug delivery system.

**Keyword:** Palm-oil esters; Nano-emulsion properties; Transdermal drug; Micelles