Thermodynamic stability, in-vitro permeability, and in-silico molecular modeling of the optimal Elaeis guineensis leaves extract water-in-oil nanoemulsion

ABSTRACT

Nanoemulsion is a delivery system used to enhance bioavailability of plant-based compounds across the stratum corneum. Elaeis guineensis leaves are rich source of polyphenolic antioxidants, viz. gallic acid and catechin. The optimal E. guineensis leaves extract water-in-oil nanoemulsion was stable against coalescence, but it was under significant influence of Ostwald ripening over 90 days at 25 °C. The in-vitro permeability revealed a controlled and sustained release of the total phenolic compounds (TPC) of EgLE with a cumulative amount of 1935.0 ± 45.7 μgcm−2 after 8 h. The steady-state flux and permeation coefficient values were 241.9 ± 5.7 μgcm−2 h−1 and 1.15 ± 0.03 cm.h−1, respectively. The kinetic release mechanism for TPC of EgLE was best described by the Korsmeyer–Peppas model due to the highest linearity of R2 = 0.9961, indicating super case II transport mechanism. The in-silico molecular modelling predicted that the aquaporin-3 protein in the stratum corneum bonded preferably to catechin over gallic acid through hydrogen bonds due to the lowest binding energies of − 57.514 kcal/mol and − 8.553 kcal/mol, respectively. Thus, the in-silico study further verified that catechin could improve skin hydration. Therefore, the optimal nanoemulsion could be used topically as moisturizer to enhance skin hydration based on the in-silico prediction.