A coarse-grained molecular dynamics study of DLPC, DMPC, DPPC, and DSPC mixtures in aqueous solution

ABSTRACT

The structural and dynamics properties of the bilayer comprising 128 molecules of dipalmitoylphosphatidylcholine (DPPC), dilauroylphosphatidylcholine (DLPC), dimyristoylphosphatidylcholine (DMPC), and distearoylphosphatidylcholine (DSPC) in water were investigated using a coarse-grained molecular dynamics (CG-MD) simulation technique. The model mixture system was simulated at 298 K under semi-isotropic pressure conditions. The aggregation was initiated from the random configurations followed by the formation of a bilayer over a period of 500 ns. The calculated values of the area per lipid, thickness, and lateral diffusion for the mixed model were different from when a single lipid was used. Our results confirmed that the chain length of the lipid molecules strongly affects the phospholipid bilayer's physical properties.

Keyword: Dipalmitoylphosphatidylcholine; Dilauroylphosphatidylcholine; Dimyristoylphosphatidylcholine, Distearoylphosphatidylcholine; Self-assembly; Coarse-grained molecular dynamics.