Investigating the effect of solvent type on the formation of Epaxal liposome (DOPC-DOPE) using coarse-grained molecular dynamics simulation

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Abstract: Liposomes or biological vesicles are formed from cholesterol and phospholipids in the aquatic environment. also sometimes other biological and non-biological molecules imported in the liposome. liposomes have a very versatile structure and thus, a variety of applications. they can be used as drug carriers and they can be “loaded” with a huge variety of molecules, as small drug molecules, proteins, nucleotides even plasmids or particles. time and process formation of liposomal systems affected by different combination of lipids. the concept of the stability and formation of liposomes is very important in the treatment of diseases and drug delivery. In this study, we are trying to investigate the effect of solvent type on the formation of epaxal liposome (DOPC-DOPE). for this purpose, a molecular dynamics simulation method is used. the analysis of the radial distribution function, solvent accessible surface area, density and radius of gyration that was performed to determine the formation and distribution of lipids, it was well demonstrated that epaxal liposome is created spherical liposome structure in a polar water environment and non-polar water environment. due to the physio-chemical properties of 1,2-dioleoyl sn-glycero-3-phosphocholine (DOPC) and 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (DOPE) phospholipids, these phospholipids tends to create a spherical liposome structure. but the type of solvent (non polar water environment) made these phospholipids in the non-polar water environment create a stretched liposome structure. according to previous articles and our findings, non-polar water is relatively polar water brings more force to the lipids, it causes the structure of the liposome to be stretched. also, because the polarity of the nonpolar solvent is low, in non-polar water, lipid molecules do not tend to accumulate together.

Keywords: liposome; molecular dynamic simulation; formation;vesicles; phospholipid

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