Formation of Polymerizable Domain in Lipid Membrane revealed by Molecular Dynamic Simulation

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Nano-delivery systems that are amenable to release drugs at desired sites have been developed since decades. Among these, intensive research has been conducted using the liposomes as triggerable drug carriers. Photopolymerizable phospholipid DiynePC (1,2-bis-(tricosa-10,12-diynoyl-sn-glycero-3-phosphocholin) is fascinating candidate for that and shows unique assembly characteristics in the lipid bilayer. Because of the presence of the diacetylene groups, DiynePC undergoes polymerization upon UV (254nm) exposure and assumes chromogenic properies. In this study, binary mixtures of two phosphatidylcholine which is composed of DiynePC and matrix lipid are simulated in bilayer state. we structurally characterize formation of polymerizable domain when DiynePC was incorporated into gel-phase matix or liquid-phase matrix.