Molecular Dynamics Simulations of the Self-Assembly of POPC Lipids

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In the last years lipsosomes have attracted increasing interest as drug delivery vehicles. The current challenge is to find a mechanism that controlls the release of the drug from the lipsosome at a specific time and location. In order to gain insight into the triggered release of nanoparticles from liposomes on a microscopic level we have performed molecular dynamics simulations. We use two different coarse grained lipid models to study the self-assembly process of POPC lipids and we observe both the formation of micelles, bicelles as well as vesicles. Comparison is made with experimental data.