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Interaction of PLGA and trimethyl chitosan modified PLGA nanoparticles with mixed anionic/zwitterionic phospholipid bilayers studied using molecular dynamics simulations[1]

BRIAN NOVAK, Louisiana State University, Center for Computation and Technology, CARLOS ASTETE, CRISTINA SABLIOV, Louisiana State University, Department of Biological and Agricultural Engineering, DOREL MOLDOVAN, Louisiana State University, Department of Mechanical Engineering — Poly(lactic-co-glycolic acid) (PLGA) is a biodegradable polymer. Nanoparticles of PLGA are commonly used for drug delivery applications. The interaction of the nanoparticles with the cell membrane may influence the rate of their uptake by cells. Both PLGA and cell membranes are negatively charged, so adding positively charged polymers such as trimethyl chitosan (TMC) which adheres to the PLGA particles improves their cellular uptake. The interaction of 3 nm PLGA and TMC-modified-PLGA nanoparticles with lipid bilayers composed of mixtures of phosphatidylcholine and phosphatidylserine lipids was studied using molecular dynamics simulations. The free energy profiles as function of nanoparticles position along the normal direction to the bilayers were calculated, the distribution of phosphatidylserine lipids as a function of distance of the particle from the bilayer was calculated, and the time scale for particle motion in the directions parallel to the bilayer surface was estimated.

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