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MOLECULAR DYNAMICS OF NANOPARTICLE TRANSPORT MECHANISM IN CELL MEMBRANES

Abstract

Understanding and measuring the cellular fate of nanoparticles in the human body is crucial to the success of drug carriers and development of vaccines against deadly toxins. Studies of the cellular uptake of nanoparticles with explicit details of transport and trafficking mechanisms in tumor cellular membranes is scarce but these studies are required to produce safe, inexpensive and effective nanomedicine and vaccines. The present study will implement molecular dynamics simulation using the CHARMM-GUI Membrane Builder and CHARMM36 lipid force field to study the transport of particles in the cell membrane. Normal plasma membranes will be modelled based on past experimental studies. The atomistic model will be set-up using headgroups of the most common phospholipids, i.e., PC (phosphatidylcholine), PE (phosphatidylethanolamine), PS (phosphatidylserine) lipids for the normal cell membranes. This study will give an insight and opportunities into developing new drug delivery vehicles and vaccines in space for the prevention of deadly toxins in the human body.