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Permeation of Beta Cyclodextrin and its Derivatives into the Lipid Membrane

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Beta cyclodextrin (βCD) and its derivatives such as methylated βCD (MEβCD) and hydroxypropyl βCD (HPβCD) have been widely used to improve the solubility and the stability of poor water soluble drugs. Most drugs are completely bound inside the hydrophobic cavity interior of the βCDs. In the present work, we studied the pre-step of drugs releasing based on drug-βCDs complexes. The interaction of three different types of βCDs i.e. βCD, 2,6-DMβCD and 2,6-HPβCD) with phospholipid bilayer was investigated using molecular dynamics (MD) simulations. The influence of chemical function groups and the orientation of βCDs interacting with bilayer surface on βCDs' permeation was studied. Our results showed that all βCDs passively adsorbed on the POPC bilayer surface via hydrogen bonding with different permeation depth and orientation. The order of permeation depth of βCDs was βCD > 2,6-DMβCD > 2,6-HPBCD. The βCD was permeated deeper when interacting with lipid bilayer by facing its secondary rim toward the bilayer's center. In contrary, the 2,6-DMβCD and 2,6-HPβCD adsorbed into the deeper part with turning its primary rim toward the bilayer's center. The molecular details of the interactions of βCDs and phospholipids are helpful to the selection of the appropriate βCDs in the pharmaceutical applications.

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