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عنوان مقاله:

Permeation of Some Terpene Derivatives through the DPPC Model Membrane: An In-Silico Study

محل انتشار:

ششمین کنگره ملی تحقیقات راهبردی درشیمی و مهندسی شیمی با تاکید بر فناوری های بومی ایران (سال: 1398)

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خلاصه مقاله:

Terpenes, the volatile components of the essential oils (Eos) consisting in many citrus fruits, mints, and herbs, are a unique group of hydrocarbon molecules, and the secondary metabolites with a key-role in plants protection. These compounds display a wide range of biological activities against cancer, malaria, inflammation, and a variety of infectious diseases.It is well knwon that for bioavailability, drugs must interact with, and eventually permeate the lipid bilayer, on the surface of the cells. Gaining a clear insight into the drug -membrane interactions is essential for an effective drug design. Molecular dynamics (MD) simulations are particularly suited to study drug-membrane systems, especially to capture interaction details on the molecular scale.This study aims to assess the permeation ability of nine terpenes, across the Dipalmitoylsphosphatidylcholine (DPPC) model membrane, through both equilibrium and non-equilibrium MD simulation approaches. First, by using an equilibrium molecular dynamics simulation, permeation of terpenes through the DPPC bilayer and their interaction with this model membrane was studied.In the next step, in order to get better sampling along the reaction coordinate and find out the free energy barrier of membrane crossing, the umbrella sampling (US) technique was employed to calculate the potential of mean force (PMF). US is one of the most efficient and reliable methods for PMF computing, based on rigorous probability calculations, along a given coordinate. Obtained results of both techniques are in good agreement with available experimental data and with each other.Direct relationship was observed between the ability of drugs to establish hydrogen bonds with the DPPC molecules, and their permeation into the head part of DPPC lipids, in the equilibrium MD simulations. On the other hand, in biased MD simulations, the compounds with more hydrogen bonds, showed greater values for free energy barrier of membrane crossing.

کلمات کلیدی:

Terpenes, Molecular Dynamics Simulation,Umbrella Sampling, Cancer, Essential oils.

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