Title:	Dynamics of heroin molecule inside the lipid membrane: a molecular dynamics study
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Abstract:	Heroin, or diamorphine (C21H23NO5), is an opium product used for various pharmaceutical and euphoric purposes. In this work, the molecular dynamics simulation study of the heroin inside the two lipid bilayers, dipalmitoylphosphatidylcholine (DMPC) and dipalmitoylphosphatidylcholine (DPPC) are presented. The whole study was conducted at three different temperatures. The location of the heroin drug, the nature of the diffusion, rotational correlation function and structural variation inside both lipid bilayers is studied. Moreover, the free energy of the solvation of the drug inside both lipid bilayers is calculated. It is found that during the whole molecular dynamics study, the drug locates at the center of both lipid membranes. The effect of the temperature is not seen at the drug location. The nature of the diffusion of the heroin drug is anomalous. The radius of gyration is calculated to study the structural variations of the heroin molecule inside both lipid bilayers. It is found that the heroin molecule does not change its structure at three temperatures. From the rotational correlation function, it is seen that the drug is more hindered for rotation inside the DPPC lipid bilayer as compared to the DMPC lipid bilayer. It is applicable for all three temperatures. The rotational correlation time of the drug is decreased while the temperature of the system is increased. In the case of DMPC, there is an abrupt change in rotational correlation time while the phase is changed.
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