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Assessment of Drug Delivery Systems from Molecular Dynamic Perspective

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Abstract : In this study, we developed and simulated nano-drug delivery systems efficacy in compare to free drug prescription. Computational models can be utilized to accelerate experimental steps and control the experiments high cost. Molecular dynamics simulation (MDS), in particular NAMD was utilized to better understand the anti-cancer drug interaction with cell membrane model. Paclitaxel (PTX) and dipalmitoylphosphatidylcholine (DPPC) were selected for the drug molecule and as a natural phospholipid nanocarrier, respectively. This work focused on two important interaction parameters between molecules in terms of center of mass (COM) and van der Waals interaction energy. Furthermore, we compared the simulation results of the PTX interaction with the cell membrane and the interaction of DPPC as a nanocarrier loaded by the drug with the cell membrane. The molecular dynamic analysis resulted in low energy between the nanocarrier and the cell membrane as well as significant decrease of COM amount in the nanocarrier and the cell membrane system during the interaction. Thus, the drug vehicle showed notably better interaction with the cell membrane in compared to free drug interaction with the cell membrane.

Keywords : anti-cancer drug, center of mass, interaction energy, molecular dynamics simulation, nanocarrier
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