سمینار هفتگی ماده چگال نرم

In silico study of H2O2 transmission through the hVDAC1 protein channel: Towards understanding the anticancer capacity of cold atmospheric plasma

Abstract

One of the differences between cancer and normal cells is the abundance of voltage-dependent anion channels (VDACs). VDAC protein channels (specially VDAC1) are over-expressed in cancer cells compared to healthy cells. They are a transporter for metabolites such as hydrogen peroxide (H_2O_2). We can examine the selectivity of cold atmospheric pressure plasmas (CAPPs) by transferring H_2O_2, created by e.g., CAPPs, to the cell interior. Up to now, the molecular level mechanism of H_2O_2 transmission through the VDAC1 channel has not been studied. In this research, we perform molecular dynamic (MD) simulations for the permeation of H_2O_2 through the hVDAC1 (one of the members of the VDAC family) on the 1,2-dioleoyl-sn-glycero-3-phosphocholine (DOPC) phospholipid bilayer (PLB). Our computational results show that the free energy barrier of H_2O_2 across the hVDAC1 is 7.03 ± 1.63 KJ mol^{-1} which is lower than for the DOPC PLB (18.92 ± 7.31 KJ mol^{-1}). In addition, we realized that Val_{20}, $Asp_{12,}$ and Asp_{19} are amino acids in the α-helix chain of the hVDAC1 channel that affect in the transmission of H_2O_2. In fact, these amino acids are more involved in the free energy barrier. This indicates that the delivery of H_2O_2 into the cell interior is more easily through the hVDAC1 channel. This study gives a better insight into the role of VDACs in the selectivity of CAPPs for cancer cell death.

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