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**HELI / Health and life science**

## **The application of Cold Atmospheric Plasma (CAP) in medicine**

M. Rezaei

*Shahid Beheshti Univ., Tehran (IR)*

### **Abstract content**

Over the past few years, the application of cold atmospheric plasma (CAP) in medicine has developed into an innovative field of research of rapidly growing importance. One promising new medical application of CAP is cancer treatment.

The therapeutic effects of CAPs are related to reactive oxygen and nitrogen species (ROS and RNS) present in the plasma. Experiments are currently showing that CAP can selectively kill cancer cells and less damage to healthy cells, but the underlying mechanisms remain unclear. Using computer simulations, we try to shed light on the mechanism of selectivity, based on Voltage dependent anion channels (VDACs). These protein channels are located on the cell membrane that carries H<sub>2</sub>O<sub>2</sub> and other active oxygen species to the inner part of the cell.

Specifically, we perform molecular dynamics simulations for the permeation of H<sub>2</sub>O<sub>2</sub> through hvdac1 (one of the members of the VDAC family) on the dioleoylphosphatidylcholine (DOPC) phospholipid bilayer (PLB). The free energy barrier of H<sub>2</sub>O<sub>2</sub> across hvdac1 is lower than for the DOPC PLB. This indicates that the delivery of H<sub>2</sub>O<sub>2</sub> into the cell interior more easily through the hvdac1 channel. Due to the abundance of this channel in cancer cells compared to healthy cells, plasma is more likely to affect cancer cells. This study gives a better insight into the role of VDACs in the selectivity of CAPs for treating cancer cells.