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MOLECULAR DYNAMICS SIMULATIONS OF OXYGEN SPECIES IN A NATIVE SKIN MEMBRANE OF INTEREST FOR PLASMA MEDICINE

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Computational modeling at the molecular or atomic scale can be very useful to obtain a better insight in plasma medicine. Different atomic scale modeling approaches can be used to study the direct interaction of plasma species with biomolecules or the consequences of these interactions for the biomolecules on a somewhat longer time scale. In this work, molecular dynamics simulations are employed to investigate the mechanisms of interactions between reactive oxygen plasma species (H_2O_2, HOO, HO and O_2) and native skin membrane from an atomistic point of view. The result of dynamic distribution study of reactive oxygen species, i.e. H_2O_2 and O_2 revealed that, these species interact with cholesterol, as one of the primary target in lipid-peroxidation of skin-lipid bilayer. Moreover, the permeability of reaction oxygen species, i.e. H_2O_2, HOO, HO, and O_2 along the skin-lipid bilayer is measured by free energy profile. The result of free energy profile shows that, these species in spite of high energy barrier easily travel throughout the membrane. Thereby, breeching the free energy barriers, these reactive oxygen species are able to permeate into the cells, accordingly inflicting oxidative stress, and might lead to apoptosis. Collectively, the insight acquired from simulations may help in better understanding of the oxidation stress at atomic level. Our simulation result provides fundamental insights into the mechanisms underlying the interactions between reactive oxygen plasma species and the skin-lipid bilayer at the atomic level.

Biography

Dharmendra Kumar Yadav has completed his PhD in Biological Science from CSIR-Central Institute of Medicinal and Aromatic Plants, Lucknow, India and Postdoctoral studies from Hanyang University Korea and University of Delhi, India. He has worked as Young Scientist at All India Institute of Medical Science Jodhpur, India. He has published more than 40 papers in reputed journals, 03 Book Chapter and US Patent. He is presently working as a Research Professor at Gachon University of Medicine and Science, Incheon city, Korea.

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