ANALYSIS OF HEAVY CHARGED PARTICLES TRACK STRUCTURES TRAVERSING MEMBRANE ION CHANNELS AND SYNAPTIC RECEPTORS

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Theoretical and experimental studies on the molecular mechanisms of central nervous system (CNS) disorders induced by ionizing radiations remains a new challenge of modern radiobiology research [1]. This issue is associated with radiation protection to cosmonauts on future long-term space missions and cancer radiotherapy. Damage to a biological target by ionizing radiation can result direct damage by ionisations and indirect damage by free-radicals produced in the condensed medium surrounding the sensitive biological target. Initial radiation-induced damage to molecular structure of neuron cells is hard to investigate experimentally at the physical and chemical stages, which are key part of radiobiological mechanisms. The Monte Carlo simulation approaches have become a main tool for describing the stochastic nature of particle track structure in nanometric volumes. An aim of this work is to evaluate nanoscale energy depositions and production of reactive chemical species in the critical sites of voltage-gated ion channels and synaptic receptors when charged particle track passing through neighborhood of these individual molecular targets. Theoretical model of Geant4-DNA Monte Carlo toolkit based on detailed description of time-space evolution of track structure, atomistic-resolution models of the molecular geometry and the mathematical algorithm of atomistic approach, has been used for this purpose. The computations were performed for protons and iron ions of different energies within range of the Bragg peak region. Our results confirm experimental findings, which suggest that NMDA and GABA(A) synaptic receptors and Na^+ ion channels belong to the most probable targets of heavy ion irradiation in neural cells. Performed theoretical simulations allow to observe and to explain at a large extent the variations of radiation-induced direct and indirect damages the different types of ion channels and synaptic receptors. Our calculated data have special importance for understanding the initial molecular damages at the synaptic level leading to further dysfunction of neuron signaling and plasticity after radiation exposure.

References

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