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Competitive interaction of hydrogen peroxide and water molecules with DNA recognition sites

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Ion beam therapy is one of the most progressive methods in cancer treatment. Studies of water radiolysis process show that under the action of ionizing irradiation in the medium of biological cell different atomic and molecular species occur. The most long-living among them are hydrogen peroxide (H_2O_2) molecules. But the role of hydrogen peroxide molecules in the deactivation of the DNA of cancer cells in ion beam therapy has not been determined yet.

In the present work competitive interaction of hydrogen peroxide and water molecules with atomic groups of non-specific (phosphate groups) and specific (nucleic bases) DNA recognition sites is investigated. Interaction energies and optimized spatial configurations of the considered molecular complexes are calculated with the help of atom-atom potential functions method and density functional theory. It is shown that hydrogen peroxide molecule can form a complex with PO_4 group (with and without sodium counterion) that is more energetically stable than the same complex with water molecule. Also the atomic groups of Adenine, Thymine, Guanine and Cytosine that are more energetically favorable to be bound by H_2O_2 rather than by H_2O molecule are determined. Moreover, spatial configurations of AT and GC base pairs stabilized much better by hydrogen peroxide rather than by water molecule are found. These configurations can occur on the pathways of opening of DNA base pairs during DNA unzipping experiments. Consequently, formation of such complexes can block genetic information transfer processes in cancer cells and can be a key factor during ion beam therapy treatment.

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