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DNA-damage by free radicals in solution P.K. BISWAS, Tougaloo College, RAMIN ABOLFATH, U. Texas at Dallas, R. RAJNARAYANAM, SUNY at Buffalo, K. CHO, U. Texas at Dallas, T. BRABEC, Ottawa U., L. PAPIEZ, U. Texas, UTSW — We employ a molecular simulation based on GROMACS-CPMD QM/MM method to study the initial damage to a fragment of DNA-molecule in the solution by ionizing radiation. We illustrate that the diatomic OH-radicals that are primary product of megavoltage ionizing radiation in water-based systems form a network of hydrogen bonds with the nearby water molecules. Our molecular simulation illustrates that the Hydrogen bonds strongly alter the relative orientation of the OH-radicals and DNA molecule. This results to an angular anisotropy in the chemical pathway and a lower efficiency in the hydrogen abstraction mechanisms than previously anticipated for identical system in the vacuum. We illustrate that the thermal fluctuations of the water molecules in the solution strongly compete with the H-abstraction that shows more energitically favorable in solution than in vacuum. As a result the chemical reaction takes place with slower rate in solution than in vacuum.

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