Abstract Submitted
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Study on the Dynamics of Gene Mutation Due to DNA Adducts

YEA NA KANG, NLCS Jeju — Density-functional theory and quantum mechanical modelling technique were used to study electronic structure of gene molecules. Using the DFT, the electron system was explained using computational simulations the progression of oxidation of DNA in nerve cells, which occurs during the enzymatic metabolism from benzo[a]pyrene to benzo[a]pyrene-7,8-dihydrodiol-9,10-epoxide(BPDE). In the process, intercalation resulted in the formation of guanine benzopyrene through binding with guanine bases in the DNA. In the DNA intercalation, thermodynamic changes were observed while the guanine benzopyrene intercalates to form an adduct which the binding causes the alteration of the structure and the abnormal replication proceeds to gene mutation. Physical properties such as optimized energy, dipole moment and electrostatic potential maps were calculated to figure out how different the values of the different atoms in a molecule affect the stability of the system. Results showed that the optimization energy of the studied molecule increased as the weight and size of molecules increased. Optimization energy of the complex G-BPDE : C and C : G(3093.631kJ/mol) showed highest among the tested samples.

Richard Kyung
CRG-NJ

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