

Abstract

DNA is a biological macromolecules that are involved in the transmission of genetic data. This macromolecule, a polymer of nucleotide subunits. The nucleotide bases adenine (A), cytosine (C), guanine (G) and thymine (T) on the steps of the ladder are macromolecules. In chemistry, the small molecules in biological systems with macromolecules called ligands interact say. The objective of the study furanoside connection to thymine, Determine the best molecular structure stable and use in DNA repair. Thymine by N1 linking to C1 sugar that is say N- glycoside bond. A number of internal and external reactions of oxygen, nitrogen oxide, alkylating agents and radiation therapy by making kinds of changes in the the basic structure particularly damaged the DNA. DNA repair mechanisms can be divided into two categories: directly and indirectly to repair restoration mechanisms. in research by using from quantum mechanical calculations, angle planar various structures nucleosides based on around the bond between sugar and nucleoside (*N*-glycosidic bond) discussed in order to find the most stable structure. also, communication between the structural parameters and data obtained from the analysis of DFT, including analysis of Atoms in molecules and Natural bond orbital discussed to be with stability of the structures. The intramolecular hydrogen bonds between the open and sugar can be said that one of the main reasons for stability of these structures.

Key words: Damaged DNA, *N*-glycosidic bond, hydrogen bonding, DNA nucleotides, DNA repair



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