The DNA duplex stability: estimation of the energy of hydrogen bonds and reactivity using TATA box as model

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The spatial structure of the DNA molecule determines the physiological and biochemical mechanisms in which this carries out its biological functions. Of particular importance to the spatial structure and stability of the double helix are the hydrogen bonds [1, 2] that join both strands in the chain. Furthermore, the chemical properties of the DNA chain significantly determine the selectivity of certain proteins. In this project the energy associated with the hydrogen bonds in chains of different number of units (from 1 to 14 base pairs) is studied, taking into account two different models: ideal not relaxed model (that obey conditions of symmetry) and ideal relaxed model (relaxed structures from the previous model). On the other hand, a first approach to the selectivity of TBP to the TATA [3] box is done by studying chemical properties of this genomic region. The study was realized under the framework of DFT [4, 5] using the code DMol3 [6] (M06-L/DN) implemented in the Materials Studio software suite [7]. From the analysis could be inferred that the average energy of hydrogen bond of the ideal not relaxed model varies periodically depending on the number of base pairs in the chain. This is related with the border effects associated with the symmetry of the system, allowing the differentiation between chains with even or odd number of base pairs. An analytical model for this development, that allows obtaining the average energy of hydrogen bond for chains of any size, is proposed. While for the ideal relaxed model, the size of the chain has influence in the average energy of hydrogen bond existing between thymine and adenine, because the presence of neighbors tends to stabilize this interaction. Finally, from the Frontier Molecular Orbitals and Fukui functions [8] can explain, from the chain of eight base pairs, the way how the binding protein interacts with the TATA box region.

References: