Weak interactions in DNA: a DFT study in CpG-island-like chains

Jorge Gutiérrez-Flores, Enrique Hernández-Lemus, Fernando Cortés-Guzmán, Estrella Ramos

Abstract

Weak interactions play a fundamental role in the stability and structure of a large number of molecules. Such is the case of the hydrogen bond and π−π stacking interactions in the deoxyribonucleic acid (DNA). This work study the effect of the number of base pairs (chain length) on both hydrogen bonds and π−π stacking, using as model GC-rich chains based on the CpG islands sequence (CpG island-like chains). We found that there is no relevant effect due to the presence of other base pairs since no significant changes in hydrogen bond and π−π stacking energies were predicted. However, anticooperative effects were observed for both hydrogen bonds and π −π stacking interactions. These results are in contrast with those of TATA-box-like chains since cooperative and additive effects were found for both hydrogen bonds and π−π stacking, respectively. Finally, based on the chemical hardness and density of states, we are able to conclude that proteins may interact easier with GC-rich chains because 8GC is less hard than 8TA and, besides, its last unoccupied levels are energetically outer than those from 8TA, delving deeper into the biological differences between the TATA box and CpG island promoter regions and shedding light on the relevance, from a biological viewpoint, of noncovalent interactions, electronic and chemical properties of the different kinds of DNA sequences. We also notice that all of our work was performed under the DFT framework included in DMol3 code (M06-L/DNP).