

Title: Interactions in guanine quadruplexes

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Date: July 2020

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In recent years, the study of DNA has been a very important focus for advancing the treatment of diseases such as cancer. This research has led in the last 30 years to the discovery of guanine quadruplexes.

This discovery has led to a new view of the structure of DNA, and new applications that may arise through the application of these guanine quadruplexes.

Guanine quadruplexes are formed as an impediment to telomere shortening, and this shortening is related to the lifespan of cells, as telomeres help to give stability to chromosomes.

The studies that have been carried out have been both computational and experimental.

The results of this work have focused on the computational information gathering of different results from articles where quantum chemistry has been used, specifically based on the density functional theory (DFT).

The work has focused on the interaction of the guanine quadruplex with monovalent and divalent cations (including transition metals), and how these give stability by studying various thermodynamic parameters, with emphasis on the formation and interaction energies between the quadruplex and the metal. In addition, the interaction energy has been analyzed in more detail from its decomposition in different terms such as Pauli repulsion, electrostatic potential, or orbital interaction.

Keywords: Guanine quadruplex, interaction energy, energy decomposition analysis, density functional theory.