Abstract

In this study, structures of some substituted azacydidine molecules were optimized by means of quantum mechanical computations using PBEKCIS methods with the 6-31g (d,p) basis set set by Gaussian09 program package. The molecular docking studies were performed using Autodock 4.2 software to discover interactions that are important in inhibitory strength of the molecules against the DNA methy tansferase enzyme. Results show that hydrogen-bonding interactions between the mentioned molecules and amino acid LYS of enzyme have a key role in this case. The best interaction energy corresponds to the interaction of azacytidine with substituent CN and amino acid LYS. Effects of various parameters such as energy gaps, electron charge densities, charge transfer, and aromaticity were investigated on interaction energies.

Keywords: Azacytidine, Molecular docking, DNA methy tansferase, LYS

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Quantum mechanical and molecular docking investigation of effect of some cytosine analogue drugs in prevention of DNA Methytransferase enzyme's function

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