عنوان مقاله:

Thermodynamic and reactivity descriptors Studies on the interaction of Flutamide anticancer drug with nucleobases: A computational view

محل انتشار:

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خلاصه مقاله:

p>In this work, the interaction between Flutamide (FLU) anticancer drug with nucleobases such as cytosine, > thymine, uracil, and adenine was studied by density functional theory (DFT) methods from a thermodynamic point of view. The Gibbs free energy (ΔG) and enthalpy (ΔH) of C-FLU, T-FLU, U-FLU and A-FLU complexes were computed and demonstrate that the stronger interaction between cytosine and FLU and the adsorption of the drug on the bases proceeds spontaneously. The negative value of ΔH indicates that the adsorption of FLU drug on the cytosine, thymine and uracil bases are exothermic, these results confirmed ΔE results. During the interaction of Flutamide drug with nucleobases, the energy levels of the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) were significantly changed. The values of the energy gap (Eg) reduced during the adsorption of the FLU drug onto bases which confirmed that the reactivity of the resulted complex increase upon adsorption. On the other hand, as a result of theoretical calculations, the values of the Eg for the Base-FLU structures in water solution are decreased in comparison to the corresponding values in the gas phase, indicating more the .reactivity of the studied complexes in the aqueous medium

کلمات کلیدی:

Density functional theory, Flutamide drug, HOMO-LUMO, chemical reactivity