عنوان مقاله:

Theoretical Study on the Interaction between ۵-Fluorouracil Anticancer Drug and Nitrosamine as a Family of Potent Carcinogenic Compounds in Different Solvents: A Quantum Chemical Study

محل انتشار:

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خلاصه مقاله:

In this research, the effect of different solvents on the stability order, binding energy and hydrogen bond (H-bond) strength of Fluorouracil-Nitrosamine (FU–NA) complex is investigated by using the density functional theory (DFT). The calculations are conducted on M۰۶-۲X/۶-۳۱۱++G(d,p) level of theory for optimization of complex geometries and their monomers. Based on the average of the calculated H-bond energies, the H-bond strength in the gas phase is higher than the solution phase and in the polar solvents are close to each other and lower than the non-polar ones. Our findings also show that when the solvent effect is applied the binding energy of complex is significantly changed. The binding energy in the solution phase is also lower than the gas phase. Therefore, the stability in the polar solvents with respect to the water as natural solvent is higher than the non-polar ones. The natural bond orbital (NBO) analysis and the Bader's quantum theory of "Atoms in Molecules" (QTAIM) are also applied to evaluate the H-bond interactions .in the selected solvents

کلمات کلیدی:

fluorouracil, Nitrosamine, Solvent effect, NBO, QTAIM-۵