عنوان مقاله:

Theoretical study of the tautomerization of Carmustine in a biological media as an anti-cancer drug

محل انتشار:

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خلاصه مقاله:

Tautomers can be defined as isomers of single molecules existing in solutions or cells. Tautomers have the ability to interchange due to numerous spontaneous arrangements of chemical bonds, unlike chirality, whose molecules represent mirror images of enantiomers of one another. Tautomerization of the carmustine mechanism as a potential anti-cancer medication was examined using the DFT method. Two conformational tautomers were identified in the structure of carmustine, and the structure of both tautomers was shown to consider the contribution of atom changes to carmustine conformation. It was possible to obtain the relative energies B۳LYP/۶-۳۱۱G++ (d,p), Aug-cc-pVDZ, and ۶-۳۱۱++g(۲d,۲p) basis sets. Calculations of the highest occupied molecular orbital (HOMO), the lowest unoccupied orbital (LUMO), and bandgap energies of structures were performed while also obtaining the electronics parameters, electrophilicity, electronegativity, softness, and hardness in order to determine the compounds' reactivity within the biological medium. Based on the results, the carmustine structure and both tautomer conformations showed stability, .but T۱ had greater stability than T۲

کلمات کلیدی:

DFT, carmustine, Tautomer, Electronic parameter, Anti-cancer