

Molecular Modeling Studies of Some Uracil and New Deoxyuridine Derivatives

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Abstract

Molecular modeling results reported in this paper are crucial in highlighting the quantitative relationship between the optimized structure and computed molecular properties related to four newly synthesized uracil derivatives with promising biological potential as anticancer bioactive agents. Moreover, 5-fluorouracil (5-FU) and its tautomers and thiouracils molecular properties are studied and correlated with their biological activities. The great medical importance of these and similar molecular systems requires research on their quantitative structure-activity relationships (QSAR) in order to further improve our knowledge about how receptor binding, selectivity, and pharmacological effects are achieved. Modeling is performed in the ground and the first singlet excited states using density functional theory (DFT) and its time-dependent extension (TD-DFT), respectively.

Journal of Chemistry - 2016, July