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Original Research Article

DFT Study, Physicochemical, Molecular Docking, and ADMET Predictions of some Modified Uridine Derivatives

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ABSTRACT

Uridine derivatives are important scaffolds of many organic substances, and are now drawing more and more interests to chemist and biochemist for the synthesis of new drugs and their pharmaceutical development. In this investigation, the optimization of uridine and its synthesized derivatives were employed density functional theory (DFT) with B3LYP/3-21G level theory to elucidate their thermal (electronic energy, enthalpy, Gibb's free energy), molecular orbital (HOMO-LUMO gap, hardness, and softness) and molecular electrostatic potential (MEP) properties. Molecular docking has been performed against 3C-like protease protein 4YOI to explore the binding mode(s) and affinity with the receptor protein of derivatives (**6-9** and **14**), which had the better antimicrobial activity. It is found that, most of the derivatives are thermodynamically stable, chemically more reactive, and show better binding affinity than the parent drug. ADMET properties were also calculated to predict the improved pharmacokinetic features of all tested derivatives. This consciousness could be useful in perceiving the functions of uridine and their derivatives, as well as the related fervidity of other chemical and quantum properties**.**

Keywords: Uridine, DFT, MEP, DOS and ADMET

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