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Anti-microbial evaluation, Experimental and Theoretical Insights into Molecular Structure, Electronic Properties, and Chemical Reactivity of (E)-2-((1H-indol-3-yl)methylene)-2,3-dihydro-1H-inden-1-one

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Abstract

The present investigation describes antimicrobial, computational, study of (E)-2-((1H-indol-3-yl)methylene)-2,3-dihydro-1H-inden-1-one (IMDHI) molecule. The spectroscopic characterization methods such 1H NMR, and 13C NMR techniques were used to confirm the structure of the (IMDHI) molecule. Antimicrobial activity of the IMDHI molecule was evaluated against two Gram-negative (E. coli & P.Vulgaris) and two Gram-positive (S. aureus & B. subtilis) bacteria whereas antifungal investigation was performed against A.Niger and C.albicans fungal species. The IMDHI molecule is found to display a strong activity against E. coli, P.Vulgaris, and, B. subtilis bacterial strains. The density functional theory (DFT) calculations were performed using the Gaussian-03 package. The B3LYP/6-31G(d,p) basis set was used for the evaluation of the molecular structure, electronic properties, and chemical reactivity properties. Ionization potential, electron affinity, electronegativity, chemical hardness and softness, global electrophilicity, and chemical potential were calculated using HOMO and LUMO energy values. To investigate the electron distribution, Mulliken atomic charges and molecular electrostatic potential surfaces were discussed.

Graphical Abstract