

Computational and Experimental Investigation of Antibacterial Properties of Some Fluorinated Thioureas

Abstract

Herein, fluorinated thioureas with various substituents (F1-F3) were synthesized and characterized spectroscopically and analytically to investigate their properties as antibacterial agents. Prior to experimental studies, Density Functional Theory (DFT) modeling was performed at B3LYP/6-31G (d,p) to complement and offer comparative overview with the experimental findings. With regards to all theoretical analyses, the Frontier Molecular Orbital (FMO) demonstrated a desirable low HOMO-LUMO gap for all three designated derivatives, particularly F1 (1.60 eV), which is consistent with its GCRDs values, namely its high electronegativity and low hardness values that corresponds to low LUMO energy, suggesting higher bacterial activity. Agar diffusion assay was used for the preliminary screening of in-vitro antibacterial activity against pathogenic Gram-positive and Gram-negative bacteria. All three derivatives successfully inhibit at least two bacterial strains (*B. cereus*, *S. aureus*), but none were able to penetrate into *E. coli*. The highest inhibition rate was exhibited by F3 at $33.33 \pm 0.71\%$ against *S. aureus*, whilst F1 only managed to gain $29.63 \pm 0.00\%$ of inhibition rate for the same bacterium. Meanwhile, the lowest penetration rate was recorded at $1.53 \pm 0.35\%$ by F2 against *B. cereus*.

Keywords

Antibacterial Agents; DFT; Fluorine; FMO; Thiourea