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Synthesis, Density Functional Theory (DFT) and Antibacterial Studies of Highly Functionalized Novel Spiropyrrolidine 4-Quinolone-3-Carboxylic Acids Derived from 6-Acetyl Quinolone

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Abstract : A series of novel 4-quinolone-3-carboxylic acid grafted spiropyrrolidines as new type of antibacterial agents were synthesized via multicomponent 1,3-dipolar cycloaddition reaction of an azomethine ylides with a newly prepared (E)-4-oxo-6-(3-phenyl-acryloyl)-1,4-dihydro-quinoline-3-carboxylic acids in high regioselectivity with good yields. The structure of cycloadduct characterized by FT IR, mass, 1H, 13C, 2D NMR techniques and elemental analysis. Structure and spectrometry of compound 8a has been investigated theoretically by using HF and DFT approach at B3LYP, M05-2x/6-31G* levels of theories. The optimized geometries and calculated vibrational frequencies are evaluated via comparison with experimental values. A good agreement is found between the measured and calculated values. The DFT studies support the molecular mechanism of this cycloaddition reaction and determine the molecular electrostatic potential and thermodynamic properties. Furthermore, the antibacterial activities of synthesized compounds were evaluated against Gram-positive bacteria (Staphylococcus aureus, Bacillus subtilis) and Gram-negative bacteria strains (Escherichia coli, Klebsiella pneumoniae). Among 21 compounds screened, 8f and 8p were found to be more active against tested bacteria.

Keywords : antibacterial activity, azomethine ylide, DFT calculation, spirooxindole
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