

Design, Synthesis, in Vitro and in Silico Characterization of 2-Quinolone-L-alaninate-1,2,3-triazoles as Antimicrobial Agents

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Abstract

Due to the growing issue of antimicrobial resistance, there is an urgent need for the development of new antimicrobial agents. Motivated by the broad antibacterial effects of various heterocyclic compounds, such as 2-quinolone derivatives, we designed and synthesized novel methyl-(2-oxo-1,2-dihydroquinolin-4-yl)-L-alaninate-1,2,3-triazole derivatives. These compounds were created through a 1,3-dipolar cycloaddition reaction between 1-propargyl-2-quinolone-L-alaninate and suitable azide groups, yielding products in good amounts (75-80%). The chemical structures of the compounds were confirmed through spectroscopic techniques, and their antimicrobial activity was tested against both bacterial and fungal strains, showing significant antibacterial effects and weak to moderate antifungal activity. Although the quinolone moiety of our compounds resembles fluoroquinolones, they do not act by inhibiting DNA gyrase. Computational studies suggest that the compounds have favorable physicochemical and pharmacokinetic properties, indicating their potential as candidates for further development as antimicrobial agents for clinical applications.

Keywords

Cycloaddition, Quinolone, Antibacterial Activity, Docking Study