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INTERNATIONAL CONFERENCE ON MULTIDISCIPLINARY STUDIES AND EDUCATION: a collection scientific works of the International scientific conference – London, England, 2026. Issue 6

Languages of publication: Uzbek, English, Russian, German, Italian, Spanish

The collection consists of scientific research of scientists, graduate students and students who took part in the International Scientific online conference **«INTERNATIONAL CONFERENCE ON MULTIDISCIPLINARY STUDIES AND EDUCATION».** Which took place in London 2026.

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REGIOSELECTIVE SYNTHESIS AND ANTIMICROBIAL SCREENING OF NOVEL S-ALKYL DERIVATIVES OF 5-(PYRIDIN-4-YL)-1,3,4-OXADIAZOLE-2-THIOL

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In medicinal chemistry, the molecular hybridization strategy—which entails merging two or more distinct bioactive pharmacophores into a single molecular entity—represents a highly effective approach to overcoming the challenges of drug-resistant pathogenic strains [1]. Both the pyridine ring (a core fragment of isoniazid) and the 1,3,4-oxadiazole heterocycle are well-recognized for their potent standalone antimicrobial and mycobacterial efficacies [2]. Consequently, structural modification at the exocyclic sulfur atom of the 5-(pyridin-4-yl)-1,3,4-oxadiazole-2-thiol scaffold, which inherently consolidates these two privileged nuclei, significantly calibrates the lipophilicity profile (log P) of the system, thereby enhancing the overall bioavailability and pharmacokinetic manageability of the potential therapeutic agent [3, 4].

The primary objective of this study is the targeted synthesis of novel S-alkyl derivatives based on isoniazid-derived 5-(pyridin-4-yl)-1,3,4-oxadiazole-2-thiol, followed by the comprehensive evaluation of their spectral parameters and the determination of their antimicrobial spectrum against specific screening test strains.

Synthetic procedures were executed via a nucleophilic substitution pathway. The starting thiol compound was initially activated at room temperature in anhydrous DMF in the presence of potassium carbonate (K_2CO_3) acting as a proton acceptor. Subsequently, short-chain aliphatic halides (methyl iodide, ethyl bromide, and propyl bromide) and an aromatic benzyl chloride were added dropwise to the reaction mixture. The underlying reaction was continuously stirred at a thermal range of 55–60 C for a duration of 4 hours. Structural elucidation of the synthesized molecules was performed utilizing FT-IR (400–4000 cm^{-1}) and UV-Vis (200–400 nm) spectroscopy techniques. The biological profiles were evaluated against Staphylococcus aureus, Escherichia coli, and Candida albicans microbial strains using standardized disk diffusion and broth microdilution methodologies.

The target reactions successfully yielded four novel hybrid S-alkyl oxadiazole derivatives with high chemical yields ranging from 70% to 85%. In the FT-IR spectra, the complete disappearance of the weak absorption band characteristic of the thiol (–SH) group at 2565 cm^{-1}—while the C=N stretching frequencies of both the pyridine (1595 cm^{-1}) and oxadiazole (1615 cm^{-1}) rings remained structurally unaltered—along with the emergence of new, intense signals typical of the C–S–C linkage in the 745–760 cm^{-1} region, rigorously confirmed that the alkylation proceeded regioselectively at the sulfur atom. The UV-Vis spectra exhibited $\pi \rightarrow \pi^*$ electronic transitions within the 254-262 nm range due to the core conjugation of the pyridine-oxadiazole network, accompanied by distinct bathochromic shifts correlated with the increasing size and lipophilic nature of the substituents.

According to the antimicrobial screening data, the integration of the pyridine nucleus enhanced the efficacy of these compounds, particularly against Gram-negative bacteria (E. coli) and fungal pathogens (C. albicans) by altering cell wall permeability. Structure-activity relationship (SAR) analysis revealed that the 2-(benzylthio)-5-(pyridin-4-yl)-1,3,4-oxadiazole derivative, which possesses the highest calculated lipophilicity coefficient, exhibited the maximum potency across all tested strains (zone of inhibition: 18–20 mm). Notably, the minimum inhibitory concentration (MIC) of this specific compound against the C. albicans strain (15.62 \mu g/mL) was fully equivalent to the clinical benchmark set by the reference antifungal drug, fluconazole.

Novel S-alkyl derivatives of 5-(pyridin-4-yl)-1,3,4-oxadiazole-2-thiol were successfully synthesized with high yields, and their spectral parameters were comprehensively validated. The hybridization of pyridine and oxadiazole architecture with targeted S-alkyl radicals was demonstrated to remarkably boost the overall antimicrobial potential. These findings provide a fundamental scientific poydevor for the targeted molecular design (drug design) of next-generation, broad-spectrum antibacterial agents based on privileged heterocyclic frameworks.

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