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REGIOSELECTIVE N-ACYLATION OF 2-MERCATOBENZIMIDAZOLE: SYNTHESIS, THERMODYNAMIC STABILITY, AND TARGETED ANTIMICROBIAL MECHANISMS

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The targeted functionalization of ambident heterocyclic systems remains a highly challenging frontier in modern medicinal chemistry and molecular design [1]. Unlike soft alkylating agents that exhibit a high affinity for the exocyclic sulfur atom, hard acylating electrophiles introduce a unique competition between kinetic S-acylation and thermodynamic N-acylation pathways within the 2-mercaptobenzimidazole core [2]. Exploring this regioselective behavior is critical because introducing structurally diverse acyl groups onto the endocyclic nitrogen atom drastically alters the electronic density distribution of the imidazole ring. This structural shift not only creates a unique electrostatic profile but also improves the capability of the compound to form precise hydrogen bonds with key bacterial and fungal enzyme pockets [3, 4].

The primary objective of this investigation is to establish an optimized protocol for the regioselective N-acylation of 2-mercaptobenzimidazole using diverse aliphatic and aromatic acyl halides, evaluate the thermodynamic stability of the resulting scaffolds via spectral characterization, and assess their in vitro antimicrobial spectrum.

Synthetic maneuvers were conducted under strict low-temperature conditions (0-5 C) in anhydrous tetrahydrofuran (THF) or dichloromethane (DCM) utilizing triethylamine (Et_3N) as a non-nucleophilic proton scavenger to trap the generated hydrogen halides. Acetyl chloride, propionyl chloride, butyryl chloride, and benzoyl chloride were sequentially employed as acylating vectors. The crude architectures were systematically analyzed using thin-layer chromatography (TLC) and purified via recrystallization. Structural validation and confirmation of the regioselective pathway were achieved through FT-IR (400–4000 cm^{-1}) and UV-Vis (200–400 nm) spectroscopy. The in vitro antimicrobial efficacy was dynamically monitored against Staphylococcus aureus, Escherichia coli, and Candida albicans using standard disk diffusion and broth microdilution (MIC) techniques.

The chemical transformations smoothly generated four distinct N-acyl-2-mercaptobenzimidazole derivatives with exceptional yields varying from 75% to 88%. The FT-IR spectral profiles provided conclusive evidence regarding the regioselectivity of the reaction. The persistent retention of the sharp, characteristic thiol/thione (S-H/C=S) stretching networks in the 2570 cm^{-1} and 1150 cm^{-1} domains, coupled with the emergence of a highly intense, downfield-shifted amide carbonyl (C=O) vibration band in the 1695–1725 cm^{-1} region, rigorously verified that the acylation exclusively manifested at the endocyclic nitrogen (N1 position). The UV-Vis absorption profiles illustrated highly diagnostic absorption maximums at 265–288 nm corresponding to modified $\pi \rightarrow \pi^*$ electronic transitions, indicating a significant delocalization of the nitrogen lone pair into the newly appended carbonyl system.

The biological screening profiles revealed that the synthesized N-acyl derivatives displayed an enhanced and highly specific antimicrobial spectrum compared to standard S-alkylated analogs. Structure-activity relationship (SAR) deconvolution indicated that the electron-withdrawing nature of the acyl scaffold significantly accentuates the acidity of the remaining thione/thiol proton, facilitating superior ionic interactions with microbial cell-wall proteins. The 1-benzoyl-1H-benzo[d]imidazole-2-thiol derivative demonstrated the most outstanding performance, generating massive zones of inhibition (20-23 mm). Its minimum inhibitory concentration (MIC) against C. albicans was recorded at a remarkable 7.81 \mu g/mL, which outperforms several classical azole benchmarks and matches the clinical standards of fluconazole.

A series of novel N-acyl-2-mercaptobenzimidazoles was successfully synthesized via a highly regioselective and thermodynamically controlled pathway. Spectral characterization confirmed the exclusive formation of N-amide linkages rather than S-esters. The notable biological efficacy observed against resistant fungal and bacterial strains underscores that N-acylation is a highly potent structural modification strategy to elevate the pharmacological profile of benzimidazole architectures. These findings lay down a robust scientific framework for the logical engineering of next-generation macromolecular enzymatic inhibitors.

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