STUDY OF HETEROCYCLIC COMPOUNDS AS ANTIMICROBIAL AGENT

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Summary

Introduction

This Ph.D. thesis encompasses a series of chapters dedicated to the synthesis of a diverse array of derivatives. These include compounds featuring oxadiazole and triazole, as well as imidazo[1,2-*a*]pyridine, and triazole-containing theophylline derivatives through click chemistry. Additionally, the work explores Schiff base formations from quinoline and thieno[2,3-*d*]pyrimidine, along with pyrazole-4-carbaldehyde containing oxime derivatives. Each chapter delves into the methodologies employed, the reaction conditions optimized, and the characterization of the synthesized compounds, highlighting their potential applications in various fields.

Chapter: 1 Synthesis and characterization of oxadiazole derivatives bearing imidazo[1,2-*a*]pyridine scaffold

This chapter details the synthesis and characterization of a broad range of 1,3,4-oxadiazole derivatives through multistep reactions. These methodologies resulted in the creation of structurally diverse compounds. Specifically, the synthesis of a novel series of 2-((5-(2-methylimidazo[1,2-*a*]pyridine-3-yl)-1,3,4-oxadiazol-2-yl)thio)-*N*-phenylacetamide derivatives starting from imidazo[1,2-*a*]pyridine is highlighted. The chapter provides comprehensive insights into the reaction procedures, emphasizing their spectral characterization using techniques such as NMR, IR, and mass spectrometry. The significance of these compounds in medicinal chemistry is also discussed, underscoring their potential applications in drug discovery and development.

Chapter: 2 Synthesis and characterization of 2-((4-amino-5-(2-methylimidazo[1,2-a]pyridin-3-yl)-4*H*-1,2,4-triazol-3-yl)thio)-*N*-phenylacetamide derivatives

This chapter focuses on the comprehensive exploration of 1,2,4-triazole derivatives, encompassing their synthesis, characterization, pharmacological activity, spectral analysis, and methodological aspects. The synthesis of these derivatives involved multistep reactions, leading to the formation of structurally diverse compounds.

The synthesis of a novel series of 2-((4-amino-5-(2-methylimidazo[1,2-*a*]pyridin-3-yl)-4*H*-1,2,4-triazol-3-yl)thio)-*N*-phenylacetamide derivatives starting from imidazo[1,2-*a*]pyridine is highlighted. The pharmacological activity of the synthesized compounds was evaluated, revealing their potential in various biological assays. Spectral characterization techniques such as NMR, IR, and mass spectrometry were employed to confirm the chemical structures. The methodologies utilized in the synthesis and characterization processes were novel, efficient, and time-effective. Overall, this chapter provides a detailed account of the synthesis, characterization, and pharmacological evaluation of 1,2,4-triazole derivatives, highlighting their potential applications in medicinal chemistry.

Chapter: 3 Synthesis and Characterization of 1,2,3-triazol containing Theophylline moiety

This chapter delves into the synthesis, characterization, and pharmacological importance of derivatives based on theophylline, 1,2,3-triazole, and employing click chemistry methodologies. A novel set of 2-(4-((1,3-dimethyl-2,6-dioxo-1,2,3,6-tetrahydro-7*H*-purin-7-yl)methyl)-1*H*-1,2,3-triazol-1-yl)-*N*-phenylacetamide derivatives involved multistep reactions to obtain a diverse range of compounds, with a focus on their structural characterization using spectral techniques such as NMR, IR, and mass spectrometry. The pharmacological importance of these derivatives was evaluated through various assays, highlighting their potential applications in medicinal chemistry. The methodology employed in this study was novel and efficient, showcasing the application of click chemistry in the development of bioactive compounds. Overall, this chapter provides a comprehensive exploration of theophylline-based 1,2,3-triazole derivatives, emphasizing their synthesis, methodology, spectral characterization, and pharmacological significance.

Chapter: 4 Synthesis and Characterization of Schiff bases derived from 2-Chloroquinoline-3-carbaldehyde and Its Derivatives

This chapter focuses on the synthesis and characterization of Schiff bases derived from 2-chloroquinoline-3-carbaldehyde and its derivatives, with a particular emphasis on incorporating 4-hydrazinyl-5,6,7,8-tetrahydrobenzo[4,5]thieno[2,3-*d*]pyrimidine in heterocyclic ring formation.

The synthetic procedures involve the reaction of 2-chloroquinoline-3-carbaldehyde with various substituted benzohydrazides to form Schiff bases. These Schiff bases were further utilized in the synthesis of novel heterocyclic compounds, particularly focusing on 4-hydrazinyl-5,6,7,8-tetrahydrobenzo[4,5]thieno[2,3-*d*]pyrimidine derivatives. The synthesized compounds were characterized using spectroscopic techniques such as NMR, IR, and mass spectrometry, and their structures were confirmed. This work contributes to the development of new heterocyclic compounds with potential applications in medicinal chemistry and pharmaceutical sciences.

Chapter : 5 Synthesis and Characterization of 3-(4-Chlorophenyl)-*N*-hydroxy-*N*,1-diphenyl-1*H*-pyrazole-4-carboximidamide derivatives

This chapter entails the synthesis and characterization of novel 3-(4-chlorophenyl)-*N*-hydroxy-N,1-diphenyl-1*H*-pyrazole-4-carboximidamide derivatives, a novel compound with potential pharmacological significance. The synthesis involves the reaction of appropriate precursors under controlled conditions to form the desired product. The synthesized compound is characterized using various spectroscopic techniques such as NMR, IR, and mass spectrometry to elucidate its molecular structure and confirm its identity. This study contributes to expanding the library of pyrazole derivatives and provides insights into their potential applications in medicinal chemistry and drug discovery.

Chapter : 6 Assessment of the Biological Activity of Newly Synthesized Compounds

This chapter presents the comprehensive biological activity evaluation of newly synthesized compounds described in chapters 1 to 5. The synthesized New Chemical Entities (NCEs) were screened for their antibacterial and antifungal activities. The compounds were evaluated using standard microbiological assays against a panel of bacterial and fungal strains. The results of the screening assays, including minimum inhibitory concentrations (MICs) and zone of inhibition (ZOI) measurements, are reported. The biological activity data demonstrate the potential of these compounds as antimicrobial agents. This study contributes valuable insights into the development of new therapeutic agents targeting bacterial and fungal infections.

Conclusion:

The present research work focused on the synthesis and characterization of a wide array of heterocyclic compounds, particularly oxadiazoles, triazoles, Schiff bases, and pyrazole derivatives. These compounds were rationally designed and synthesized using well-established synthetic protocols. Structural confirmation was achieved through IR, 1H NMR, 13C NMR, and mass spectrometric techniques, ensuring the authenticity and purity of the synthesized molecules.

Biological evaluation of the synthesized compounds revealed promising antimicrobial potential, especially against common bacterial and fungal strains. Several derivatives demonstrated significant activity comparable to standard drugs, indicating their potential as lead candidates in drug discovery. The structure–activity relationship (SAR) studies further supported the influence of specific functional groups and molecular frameworks on bioactivity.

Overall, the research not only contributes to the growing body of knowledge in heterocyclic medicinal chemistry but also opens avenues for further optimization and exploration of these scaffolds for pharmaceutical applications. The insights gained through this work provide a strong foundation for future drug development and pharmacological research.