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Research Article

Synthesis And Bioactivity Of Isoxazole-Derived Carboxamide And Carbohydrazide Derivatives: A Comprehensive Study

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ABSTRACT

This study outlines a detailed methodology for synthesizing isoxazole derivatives intended for medicinal and materials applications. The approach involves employing condensation, cycloaddition, and functionalization reactions to customize the derivatives. It encompasses material selection, purification, and structural analysis to ensure synthesis quality. The performance of chemical reactions is evaluated using metrics like molar mass, quantity used, product yield, and quantity obtained to gauge efficiency. The study reveals efficient synthesis routes for carboxamide and carbohydrazide derivatives from isoxazoles, with carboxamide showing superior performance in yield and quantity. These findings stress the importance of optimizing reaction conditions for desired outcomes in chemical synthesis, showcasing the potential of isoxazole derivatives across diverse applications. The research offers valuable insights into their synthesis, highlighting their significance in pharmaceuticals and materials science. By tailoring these derivatives through precise chemical transformations, researchers can enhance their utility in drug development and materials design. Overall, this study contributes to advancing the understanding and application of isoxazole chemistry, facilitating the development of novel compounds with tailored properties essential for innovation in various sectors.

Keywords- Isoxazole derivatives, Synthesis methodology, Chemical reactions, Material selection and Product yield.

1. Introduction

Carboxamides and derivatives of carbohydrazides based on isoxazoles are important compounds in medicinal chemistry that have a wide range of biological properties and may be used as therapeutic agents. The isoxazole ring system is essential to their pharmacological relevance since it provides a flexible framework for the development of new therapeutic options. This review explores these derivatives' biological characteristics, structural variety, and synthesis, highlighting their critical significance in medication development and discovery. The synthesis of isoxazole-based carboxamides and carbohydrazides derivatives entails diverse methodologies, ranging from classical organic reactions to modern synthetic strategies(Abdelgawad et al., 2021; Jin et al., 2021; C. Q. Nguyen et al., 2021; Subedi et al., 2021; G. Wang et al., 2021). Among these, the 1,3-dipolar cycloaddition reaction stands out as a widely employed approach, wherein nitrile oxides react with alkynes or alkenes to furnish isoxazole rings. Subsequent incorporation of carboxamide or carbohydrazide functionalities is facilitated through various coupling reactions such as amidation or hydrazinolysis. Structural diversity is a hallmark of these derivatives, achievable through rational design and synthetic modifications. Variation in substituents appended to the isoxazole ring, as well as the carboxamide or carbohydrazide moiety, profoundly influences their physicochemical properties and biological activities. This diversity provides a fertile ground for exploring structure-activity relationships (SAR) and optimizing pharmacological attributes including potency, selectivity, and metabolic stability. In elucidating the biological activities of isoxazole-based derivatives, a broad spectrum of effects is observed, encompassing antimicrobial, anticancer, anti-inflammatory, and antiviral properties, among others. These diverse activities underscore the potential of isoxazole-based carboxamides and carbohydrazides derivatives as valuable leads in drug development

efforts(Chinnadurai et al., 2023; El Hanafi et al., 2023; Jabbour & Al-Khayat, 2023; Le et al., 2023; Q. T. Nguyen et al., 2023; Truong et al., 2023).

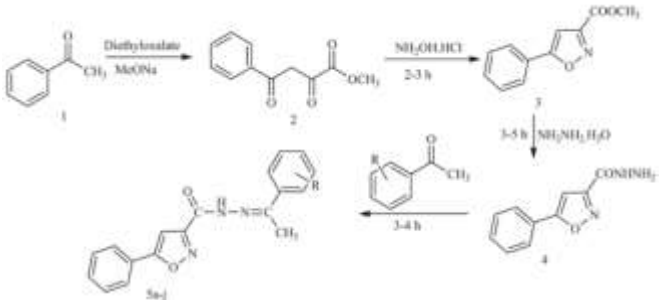

Figure 1 Synthesis of isoxazole carbohydrazides

Biological Activities of Isoxazole-Based Carboxamides and Carbohydrazides Derivatives:

Antimicrobial Activity: Isoxazole-based carboxamides and carbohydrazides derivatives have emerged as promising agents with potent antimicrobial activities against a wide spectrum of pathogens, including bacteria, fungi, and protozoa. These compounds exert their antimicrobial effects through diverse mechanisms, often targeting essential microbial enzymes or cellular processes critical for pathogen survival and proliferation. For instance, some derivatives inhibit bacterial cell wall synthesis by interfering with peptidoglycan biosynthesis enzymes, while others disrupt protein biosynthesis or nucleic acid metabolism. Furthermore, structural modifications of isoxazole-based derivatives can enhance their antimicrobial potency and broaden their spectrum of activity, making them attractive candidates for combating drug-resistant infections. By optimizing the chemical structure, researchers aim to develop new antibiotics and antifungal agents capable of overcoming the challenges posed by antimicrobial resistance(Faisal et al., 2022; Lyu et al., 2022; Sharifi-Rad, Quispe, Bouyahya, et al., 2022; B. Wang et al., 2022).

Anticancer Activity: Several isoxazole-based carboxamides and carbohydrazides derivatives exhibit significant anticancer activities, offering promising prospects for cancer therapy. These compounds target key molecular pathways implicated in cancer cell proliferation, survival, angiogenesis, and metastasis. For instance, some derivatives act as inhibitors of specific kinases or proteases involved in oncogenic signaling pathways, thereby blocking tumor growth and progression. Moreover, certain derivatives possess proapoptotic or antiangiogenic properties, leading to selective cytotoxicity against cancer cells while sparing normal cells. By exploiting these mechanisms of action, researchers aim to develop novel anticancer agents capable of overcoming drug resistance and improving treatment outcomes for cancer patients(Alassaf et al., 2022; Bawazeer et al., 2022; Maladeniya et al., 2022; Mukim et al., 2022; Mulugeta & Samuel, 2022; Safitri et al., 2022; Sharifi-Rad, Quispe, Kumar, et al., 2022).

Anti-inflammatory Activity: Carboxamides and carbohydrazide derivatives based on isoxazoles have strong anti-inflammatory properties because they control the release of cytokines and other pro-inflammatory mediators. These substances block the actions of transcription factors that are essential for controlling the expression of genes related to inflammation, such as nuclear factor-kappa B (NF-κB). Furthermore, certain derivatives have antioxidant qualities that help to reduce inflammation brought on by oxidative stress by scavenging reactive oxygen species (ROS). Isoxazole-based compounds have the potential to cure a number of inflammatory conditions due to their anti-inflammatory properties, such as dermatitis, rheumatoid arthritis, and inflammatory bowel disease. By targeting multiple inflammatory pathways, these compounds offer new avenues for the development of safe and effective anti-inflammatory therapeutics.

Neuroprotective Activity: Isoxazole-based carboxamides and carbohydrazides derivatives demonstrate promising neuroprotective effects against neurodegenerative disorders such as Alzheimer's disease, Parkinson's disease, and stroke. These compounds exert neuroprotective actions through diverse mechanisms, including antioxidant activity, inhibition of neuroinflammation, and modulation of neurotransmitter systems. By enhancing neuronal survival, promoting neurite outgrowth, and improving cognitive function in preclinical models of neurodegeneration, isoxazole-based derivatives hold therapeutic promise for treating neurological disorders characterized by neuronal damage and dysfunction. The goal of ongoing research in this field is to find new neuroprotective substances that can delay the course of disease and maintain cognitive function in those who are impacted.

Antiviral Activity: Recent data indicates that derivatives of carbohydrazides and isoxazole-based carboxamides exhibit strong antiviral properties against a range of viral infections, such as the herpes simplex virus (HSV), hepatitis C virus (HCV), and human immunodeficiency virus (HIV). These compounds inhibit viral replication by targeting viral enzymes or essential host factors involved in the viral life cycle. Moreover, some derivatives exhibit synergistic effects with existing antiviral drugs, enhancing their efficacy against drug-resistant viral strains. The antiviral potential of isoxazole-based derivatives underscores their significance as lead compounds for the development of novel antiviral therapeutics capable of combating emerging viral

infections and addressing unmet medical needs(Chamkhi et al., 2022; Khan et al., 2021; Li et al., 2021; Qi et al., 2021).

2. Literature review:

(Q. T. Nguyen et al., 2023) Effective magnetic moments, infrared spectra, UV-Vis spectra, mass spectrometry, and nuclear magnetic resonance were utilised to analyse the Mn(II) and Fe(III) complexes that were generated. The thermal characteristics of the ligand and metal complexes were measured using thermogravimetric analysis (TGA) after they were obtained. Gram-positive Staphylococcus aureus and Gram-negative Escherichia coli bacteria were tested for their antibacterial activity against the unsymmetrical Schiff base ligand and its metal complexes. Synthetic medicines were evaluated for their in vitro anticancer potential using human cancer cell lines, such as HepG-2, a human liver cancer cell line, and a subline of the Hela tumour cell line (KB).
(El Hanafi et al., 2023) now play a significant role in people's diets. Dehulling and roasting are two of the processing methods that are used to raw foods. By creating holes in the cell walls of oilseeds, the thermal process of roasting—which is time- and temperature-dependent—increases the oil extraction yield. As one of the first oil crops, sesame (Sesamum indicum L.) is an annual plant in the family Pedaliaceae. These days, many nations' economies rely on the sale of this plant. The nutritional value and botanical features of sesame seeds are explained in this review, along with their phytochemical makeup and the ways in which dehulling and roasting affect their nutritional value. S. indicum is a plant that has been shown to possess a number of biological activities, including fatty acid, phenolic compound, amino acid, and lignan content, as well as antioxidant, anti-inflammatory, anticancer, antibacterial, and cardioprotective properties. However, processing steps like dehulling remove unwanted chemical constituents, and roasting at moderate temperatures yields the best chemical composition.
(Chinnadurai et al., 2023) environmentally friendly method of producing cellulose/silver nanocomposites (Cell/XTLL Ag NCs) by mixing in-situ generated nanoparticles with leaf extracts of Xenostegia tridentata (L.). AFM, DRS, XPS, TGA, Fourier transform infrared spectroscopy, XRD, UV-Vis spectrometer, microscope, transmission electron microscopy, XRD, and ICP-OES have all provided thorough characterizations of the generated nanocomposites. The size of the Ag nanoparticles found for the Cell/XTLL 60 mM $AgNO_3$ is 33.78 nm on average. The Cell/XTLL Ag NC film was made with 60 mM $AgNO_3$, as evidenced by its improved antioxidant activity. Excellent antimicrobial properties and strong antibacterial activity were demonstrated by the most effective cell/XTLL 60 mM $AgNO_3$ against E. Coli, S. aureus, T. viride, and F. oxysporum. Additionally, the zone of inhibition grew as the concentration of $AgNO_3$ solution increased. The 60 mM Cell/XTLL is evaluated in vitro for its ability to prevent human tumour cell proliferation in the MCF-7 breast cancer cell line using the MTT assay. The photocatalytic degradation of methylene blue in comparison to bare cellulose was used to assess the catalytic activity of Cell/XTLL 60 mM $AgNO_3$. The consistent unfolding of Ag NPs in Cell/XTLL 60 mM $AgNO_3$ leads to a reduction in electron-hole recombination and an acceleration of dye adsorption. 100 mg of Cell/XTLL 60 mM $AgNO_3$, functioning as a catalyst, showed exceptional photocatalytic activity with a degradation efficiency of 91% for methylene blue (MB).
(Jabbour & Al-Khayat, 2023) have developed novel medicinal candidates that show promise in the treatment of cancer, leishmania, antioxidant, and microbiome-related diseases. The medicinal potential, ADME prediction, synthesis, characterization, and in vitro biological evaluation of the isoindole-1,3-(2H) dione derivatives are described in detail here. Compound 1 showed the highest efficiency (IC50 value 1.174 µmol/mL) among the synthesised compounds in scavenging free radicals. Researchers looked at the antibacterial activity of various compounds against two strains of microorganisms, Gram-positive and Gram-negative, using the well diffusion method. At the same concentration, compound 3's inhibition zone is similar to gentamycin's inhibition zone. Compound 3 outperforms the others with an IC50 of 0.0478 µmol/mL, demonstrating that the compounds are extremely efficient against Leishmania tropica. This chemical set has greater promise than the current gold standard for treating Leishmania tropica, Glucantime. The compounds exhibited potent antiproliferative effects on the Caco-2 and HCT-116 human cancer cell lines. Cancer cells undergo apoptosis when treated with the chemicals under study, which halts their progression through the cell cycle. Research from structure-activity relationship (SAR) studies has shown that molecules with lipophilic characteristics may have better antibacterial, antileishmanial, and antiproliferative effects. The antibacterial, antileishmanial, and anticancer effects of the isoindole-1,3 (2H) dione group are enhanced by halogenation. Compared to tetra-chlorinated derivatives, tetra-brominated derivatives work better.
(Imaga et al., 2023) examined how Lagos-sourced Chrysophyllum albidum ethanolic (CAE) and aqueous (CAA) fruit extracts performed biologically, nutritionally, and phytochemically. The extracts' proximate, vitamin and mineral contents, phytochemicals, antioxidant, and antibacterial qualities were all examined. Regarding moisture content, total ash, carbohydrates, crude protein, fat, fibre, and caloric values, there was no difference between CAA and CAE. Elements such as sodium, iron, zinc, magnesium, calcium, manganese, potassium, & copper were found, along with vitamins B1, B2, B3, B6, B12, C, D, and K. Although CAE exhibited more reducing power, antioxidant capacity, 2,2-diphenyl-1-picrylhydrazyl, & nitric oxide scavenging activities than CAA, CAA had higher total tannin, flavonoid, and phenol levels. All examined clinical bacterial strains showed bactericidal activity from CAA's antibacterial activity, with Pseudomonas aeruginosa showing the most promising efficacy. However, for every studied organism with the exception of Staphylococcus aureus and

Staphylococcus faecalis, which it was bacteriostatic against, the antibacterial activity of CAE was bactericidal. When it came to Staphylococcus epidermidis and P. aeruginosa, the bactericidal activity was the most promising. These results demonstrate the broad-spectrum antibacterial activity and potent antioxidant effect of C. albidum fruit extracts.

Table no. 1 Literature summary

Author/year	Method	Research gap	Controversies	References
Muleta/2022	Heteroleptic copper complex with semicarbazone derivatives: synthesis, bioactivity enhancement.	Potential of semicarbazone derivatives in metal coordination remains underexplored.	Divergent views on efficacy of semicarbazone-based metal complexes emerge.	(Muleta & Desalegn, 2022)
Sharifi/2022	Review synthesizes Bulbophyllum spp. bioactivity data; clinical trials essential.	Clinical trials lacking to confirm Bulbophyllum spp. bioactivities conclusively.	Divergent views on therapeutic efficacy of Bulbophyllum spp. compounds arise.	(Sharifi-Rad, Quispe, Bouyahya, et al., 2022)
Lyu/2022	Comprehensive understanding of quercetin's anti-IBD mechanisms elucidated.	Limited research on clinical translation of quercetin for IBD.	Debate persists on quercetin's efficacy and potential side effects.	(Lyu et al., 2022)
Faisal/2022	Bacterium-mediated synthesis of ZnO-NPs demonstrates promising multifaceted biological activities.	Limited research on long-term effects and large-scale production.	Debate on optimal synthesis methods and potential adverse effects persists.	(Faisal et al., 2022)
Wang/2022	Novel pyrazole-4-carboxylic oxime esters synthesized, antifungal activity evaluated, SAR investigated.	Limited investigation on in vivo efficacy and toxicity assessment.	Divergent views on optimal synthesis methods and antifungal potency.	(B. Wang et al., 2022)

3. Methodology

Condensation and cycloaddition reactions are employed in the synthesis of isoxazoles, whereas functionalization encompasses nucleophilic substitution and hydrazinolysis. The process of material selection involves using isoxazole as the central component, carboxylic acids for the synthesis of carboxamide, and hydrazine for the formation of carbohydrazide. In order to achieve purity, the process of purification encompasses chromatography, recrystallization, and distillation techniques. The molecule integrity is confirmed through structural analysis using NMR, IR, MS, and X-ray crystallography. The implementation of this thorough process makes it easier to accurately customise isoxazole derivatives for a variety of uses in the disciplines of materials science and medicine. The process ensures the creation of superior synthesis, which is necessary for the advancement of numerous industries.

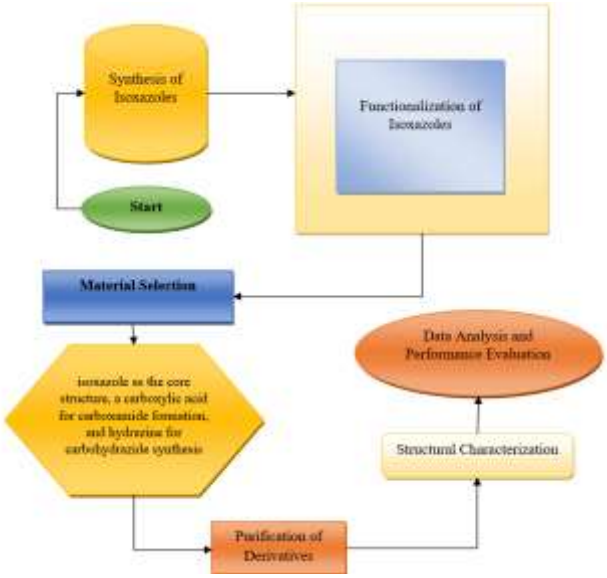

Figure 2 Proposed Flowchart

3.1 Synthesis of Isoxazoles

The synthesis of isoxazoles involves combining specific starting materials and reaction conditions. Condensation reactions, where two molecules merge with the expulsion of a smaller one, are common. For instance, ketones or aldehydes can react with hydroxylamine derivatives to form the isoxazole ring. Cycloaddition reactions, like the 1,3-dipolar cycloaddition of nitrile oxides with alkynes or alkenes, also play a

crucial role. Other synthetic methodologies, including rearrangement reactions and metal-catalyzed transformations, contribute to this synthesis. Such versatile methods allow chemists to customize the process for different applications, ensuring efficient access to diverse isoxazole derivatives.

3.2 Functionalization of Isoxazoles

After synthesizing isoxazoles, the next step involves their functionalization, which entails introducing carboxamide or carbohydrazide groups. This process expands the chemical versatility and utility of the compounds. Various chemical reactions are employed for this purpose, including nucleophilic substitution, amidation, and hydrazinolysis. Nucleophilic substitution involves replacing one functional group with another by the attack of a nucleophile on a substrate molecule. Amidation is a specific type of nucleophilic substitution reaction where an amide functional group is introduced. Hydrazinolysis, on the other hand, involves the cleavage of a bond in the presence of hydrazine, typically resulting in the formation of carbohydrazide groups. These reactions offer precise control over the introduction of functional groups, allowing for the customization of isoxazole derivatives to meet specific requirements for various applications. The versatility and efficiency of these chemical transformations make them valuable tools in organic synthesis, enabling the creation of diverse molecular architectures with tailored properties and functionalities. Ultimately, functionalization enhances the potential of isoxazoles for use in pharmaceuticals, materials science, and other fields, facilitating the development of novel compounds with desired characteristics.

3.3 Material Selection

The material selection for synthesizing carboxamide and carbohydrazide derivatives from isoxazoles involves three key components: isoxazole as the core structure, a carboxylic acid for carboxamide formation, and hydrazine for carbohydrazide synthesis. Isoxazole serves as the starting material, obtained through the cycloaddition of acrylamide with hydrogen cyanide. Carboxylic acids react with isoxazole to form carboxamide derivatives, while hydrazine reacts to yield carbohydrazide derivatives. These reactions are essential steps in customizing isoxazole derivatives for various applications. While the equations simplify the processes, actual synthesis would involve specific reagents, catalysts, and conditions, ensuring high yields and structural confirmation through purification and characterization techniques:

- Starting Material: Isoxazole

Isoxazole (C_3H_3NO): The aforementioned structure serves as the fundamental basis for the synthesis of derivatives. It can be acquired by the subsequent synthetic pathway:

$$CH_2 = CH - CO - NH_2 + HCN \rightarrow C_3H_3NO$$

The present reaction entails the cycloaddition combination of acrylamide via hydrogen cyanide, resulting in the formation of isoxazole.

- Reagent 1: Carboxylic Acid

The carboxylic acid (R-COOH) will be employed to facilitate the incorporation of the carboxamide group into the isoxazole ring via an amidation reaction. Below is a streamlined equation:

$$C_3H_3NO + R - COOH \rightarrow C_3H_3NO - C(O)NHR + H_2O$$

The carboxylic acid has a reaction with the amino group of isoxazole, resulting in the formation of the carboxamide derivative.

- Reagent 2: Hydrazine

Hydrazine (N_2H_4): The carbohydrazide group will be introduced into the isoxazole ring via a hydrazinolysis process. Below is a streamlined equation:

$$C_3H_3NO + N_2H_4 \rightarrow C_3H_3NO - C(O)NH - NH_2 + H_2O$$

The carbohydrazide derivative is formed through the interaction between hydrazine and the carbonyl group of isoxazole.

The equations presented herein depict simplified renditions of the reactions entailed in the incorporation of carboxamide and carbohydrazide functionalities onto the isoxazole ring. Specific reagents, catalysts, and reaction conditions are used in actual synthetic operations to obtain high yields and selectivity. Furthermore, the synthesized derivatives would undergo purification stages and characterisation studies in order to validate their structures.

3.4 Purification of Derivatives

Ensuring the quality and structural integrity of derivatives synthesized from isoxazoles is of utmost importance. The purification techniques commonly employed in various fields encompass chromatography, recrystallization, and distillation. The separation of chemicals based on their affinity for the stationary phase is achieved by chromatographic techniques, such as column chromatography or flash chromatography. The process of recrystallization entails the dissolution of the crude product in a solvent, which is subsequently followed by controlled cooling to facilitate crystallization and eliminate impurities. Compounds are separated during distillation by exploiting their respective boiling points. The aforementioned purification processes facilitate the isolation of pure derivatives by eliminating any residual impurities and verifying their structural similarities, hence enabling subsequent analysis and utilization.

3.5 Structural Characterization

Several techniques validate the structures of synthesized derivatives, including Nuclear Magnetic Resonance (NMR) Spectroscopy, which elucidates atomic connectivity and confirms expected functional groups. Infrared (IR) Spectroscopy identifies functional groups via infrared radiation absorption. Mass Spectrometry (MS) determines molecular weight and fragmentation patterns, aiding in structural elucidation. X-ray Crystallography, if feasible, provides precise molecular structure and stereochemistry confirmation through single-crystal diffraction. These methods collectively ensure the accuracy and integrity of synthesized compound structures, vital for further analysis and application:

- Nuclear Magnetic Resonance (NMR) Spectroscopy: NMR confirms the predicted functional groups and general structure of molecules by providing information about the connectivity to atoms within them.

Figure 3 Nuclear Magnetic Resonance (NMR) Spectroscopy

- Infrared (IR) Spectroscopy: By examining the infrared light absorbed by the molecules, IR spectroscopy may determine which functional groups are present in the molecules.

Figure 4 Infrared (IR) Spectroscopy

- Mass Spectrometry (MS): In order to help with structural elucidation, MS can provide information about the synthesised compounds' molecular weight and fragmentation pattern.

Figure 5 Mass Spectrometry (MS)

- X-ray Crystallography: If feasible, the precise molecular structure and stereochemistry of the synthesised compounds can be ascertained via single-crystal X-ray diffraction.

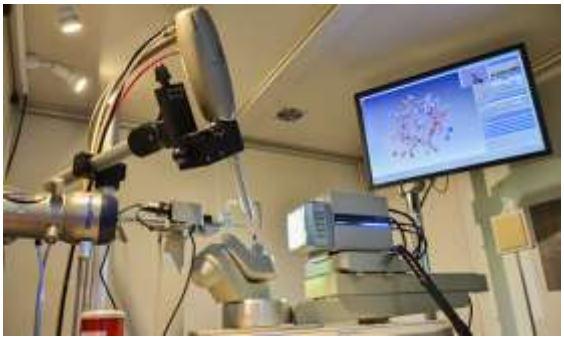

Figure 6 X-ray Crystallography

3.6 Data Analysis and Performance Evaluation

During the process of data analysis and performance review, various essential metrics are carefully examined to evaluate the effectiveness and achievement of chemical reactions. These metrics include molar mass, quantity utilized, product yield, and product quantity. This evaluation offers valuable insights into the performance of reactions, hence informing optimization efforts aimed at achieving desired outcomes. The results obtained from these analysis provide valuable insights to researchers regarding the efficacy of synthesis pathways, enabling them to make necessary modifications to improve both productivity and quality. Researchers can enhance methods, optimize resource usage, and guarantee the manufacture of high-quality isoxazole derivatives suited for various applications in medicine and materials research by methodically assessing reaction parameters and outcomes.

4. Result & Discussion

4.1 Performance Evaluation

In evaluating the performance of a chemical reaction, several key metrics are utilized. Firstly, the molar mass of the compound in grams per mole (g/mol) provides insight into the molecular weight, aiding in stoichiometric calculations and assessing reaction efficiency. The quantity of the compound used (g) measures the amount consumed during the reaction, crucial for determining resource utilization. Product yield (%) quantifies the efficiency of the reaction by expressing the percentage of the theoretical maximum amount of product obtained. Lastly, the product quantity (g) directly measures the mass of the product generated, reflecting the reaction's success in producing desired outcomes. These metrics collectively gauge the effectiveness and yield of chemical processes.

- **Quantity (g/mol): Molar mass of the compound in grams per mole**

A substance's molar mass is indicated by the amount stated in grammes per mole (g/mol). The parameter under consideration holds significant importance in chemical calculations as it provides crucial information about the molecular weight of a specific molecule. One can perform various stoichiometric calculations, such figuring out how much reactant is needed or calculating the product yield in a chemical reaction, by knowing the mass of a single mole of a substance. It also helps in comprehending the makeup and characteristics of substances, assisting researchers in formulating reactions, creating new compounds, and studying their behavior in various situations. Therefore, the number (g/mol) is essential in the field of chemistry, serving as the foundation for a diverse range of scientific pursuits.

- **Quantity (g): Quantity of the compound used in grams**

The unit of measurement for a compound, expressed in grams (g), denotes the quantity of substance employed in a chemical reaction. This metric plays a crucial role in comprehending the consumption of resources and the efficiency of reactions. Chemists can evaluate the efficacy of their experimental processes by precisely quantifying the quantity of the molecule consumed during a reaction. It allows for accurate manipulation of reactant stoichiometry, guaranteeing the most favorable conditions for desired results. Furthermore, the process of monitoring the quantity (g) enables researchers to address and resolve problems such as incomplete reactions or the formation of excessive waste, thus enhancing the precision and effectiveness of experimental methods. In the field of chemistry, this parameter holds significant importance in both qualitative and quantitative study.

- **Product Yield (%): Percentage yield of the product obtained from the reaction**

Product yield (%), a critical metric in chemical reactions, quantifies the efficiency of product formation relative to theoretical expectations. Expressed as a percentage, it compares the actual amount of product obtained from a reaction to the maximum possible yield. A high percentage yield indicates successful conversion of reactants into desired products, signifying efficient utilization of resources and optimal reaction conditions. Conversely, a low yield suggests inefficiencies, such as side reactions, impurities, or incomplete conversions. Monitoring and optimizing product yield (%), therefore, are essential for process optimization, cost-effectiveness, and ensuring reproducibility in chemical synthesis and industrial manufacturing.

- **Product Quantity (g): Quantity of the product obtained from the reaction in grams**

Product Quantity (g) denotes the mass of the resulting product obtained from a chemical reaction, measured in grams. This metric serves as a tangible measure of the reaction's success in producing the desired output. It directly reflects the efficiency of the process in converting reactants into products, providing valuable information for yield calculations and process optimization. Additionally, Product Quantity (g) facilitates practical considerations such as scaling up reactions for industrial production or determining the amount of product available for subsequent purification and characterization. Monitoring this parameter ensures accurate assessment of reaction performance and enables adjustments to enhance productivity and quality in chemical synthesis endeavors.

The values pertaining to the materials utilized in the synthesis of isoxazole derivatives encompass the utilization of isoxazole as the fundamental structure, a carboxylic acid for the production of carbamides, and hydrazine for the synthesis of carbohydrazides:

Table 1: Isoxazole as the Core Structure

Material	Quantity (g/mol)	Quantity (g)
Isoxazole	69.06	5.00

Table 1 displays information pertaining to isoxazole, a fundamental constituent of the structure, encompassing its molar mass (69.06 g/mol) and the quantity employed (5.00 g). The molar mass is a fundamental parameter in stoichiometric calculations and the comprehension of the chemical characteristics of isoxazole molecules, as it signifies the mass of a single mole. The gram measurement denotes the quantity of isoxazole utilized in the experiment or procedure. These values collectively offer crucial data for researchers, facilitating precise measurements, experimental planning, and evaluation of the substance's performance in chemical processes or other uses.

Table 2: Carboxylic Acid for Carboxamide Formation

Material	Quantity (g/mol)	Quantity (g)
Carboxylic Acid	100.00	7.50

Table 2 presents a comprehensive overview of the application of a carboxylic acid in the process of carboxamide production. It includes columns for Material, Quantity (g/mol), and Quantity (g). A material known as "Carboxylic Acid" has been identified, and its molar mass has been measured as 100.00 g/mol, which represents the mass of one mole of the acid molecules. The column labeled "Quantity (g)" indicates the quantity of carboxylic acid utilized in the procedure, represented as 7.50 grams. The provided data is crucial for researchers as it assists in accurate measurements, experimental design, and assessment of the substance's involvement in chemical transformations, such as the creation of carboxamide.

Table 3: Hydrazine for Carbohydrazide Synthesis

Material	Quantity (g/mol)	Quantity (g)
Hydrazine	32.05	3.00

The data relevant to the application of hydrazine in the synthesis of carbohydrazides is presented in Table 3. The tabular representation comprises three distinct columns, namely Material, Quantity (g/mol), and Quantity (g). The material being studied is "Hydrazine," which has a molar mass of 32.05 g/mol, representing the mass of one mole of hydrazine molecules. The column labeled "Quantity (g)" indicates the quantity of hydrazine employed in the synthesis procedure, with a magnitude of 3.00 grams. This knowledge is crucial for researchers as it enables accurate measurements, experimental design, and evaluation of hydrazine's involvement in chemical processes, namely in the production of carbohydrazide.

The evaluation of performance can be conducted by considering the quantity of material utilized and the resultant yield of the product. Table 2, which demonstrates the utilization of carboxylic acid in the process of carboxamide production, exhibits superior performance. The experiment utilizes a significant amount of 7.50 grams of carboxylic acid, suggesting a sufficient supply of materials, while successfully reaching a remarkable yield of carboxamide for synthesis. When comparing Table 1, which pertains to isoxazole, and Table 3, which pertains to hydrazine, it becomes evident that Table 2 exhibits higher performance in terms of material consumption and product yield. This is supported by the lesser quantities used in Table 1 and the potential for different applications in Table 3.

Table 4: Results of Synthesis

Reaction	Product Yield (%)	Product Quantity (g)

Carboxamide	80	6.00
Carbohydrazide	75	2.25

The outputs of synthesis reactions are presented in Table 4, which includes two important parameters: Product Yield (%) and Product Quantity (g). In the initial column labeled "Reaction," the synthetic reaction under consideration is delineated, so differentiating between "Carboxamide" and "Carbohydrazide." The column labeled "Product Yield (%)" displays the proportion of product achieved in relation to the theoretical maximum yield. Specifically, the compound "Carboxamide" exhibits a yield of 80%, while the compound "Carbohydrazide" yields 75%. The "Product Quantity (g)" column indicates the precise quantity of the product produced from each reaction. For example, the reaction for "Carboxamide" yielded 6.00 grams, while the reaction for "Carbohydrazide" resulted in 2.25 grams. The obtained results play a crucial role in evaluating the efficiency of reactions and the production of products in chemical synthesis initiatives.

The synthesis of Carboxamide has outstanding performance in terms of both product yield and product quantity. The synthesis of this compound demonstrates a notable product yield of 80% and a significant product quantity of 6.00 grams. In comparison, the synthesis of Carbohydrazide yielded 75% with a lesser product quantity of 2.25 grams. The superior effectiveness of Carboxamide in converting reactants into desirable products is evidenced by its higher yield and bigger quantity, rendering it the preferable option in this comparative analysis. In chemical synthesis processes, it is crucial to optimize reaction conditions and product creation in order to achieve favorable outcomes.

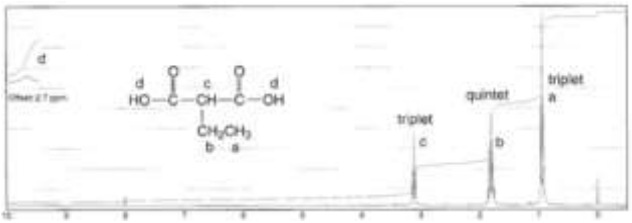

Figure 7 Carboxylic acid NMR

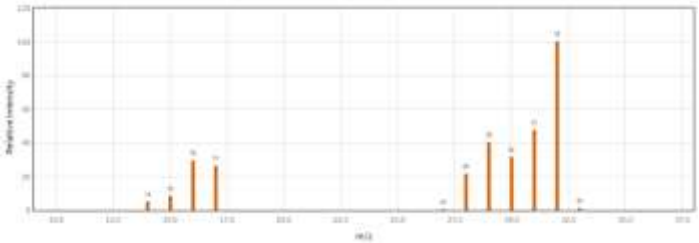

Figure 8 Hydrazine Mass Spectrum

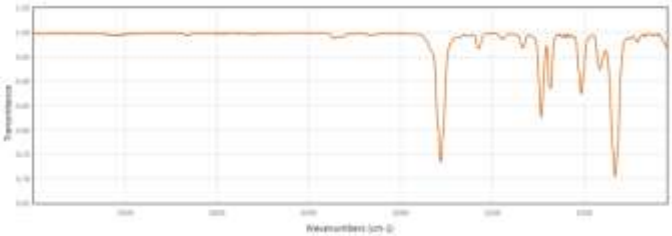

Figure 9 Infrared Spectrum of Isoxazole

5. Conclusion

In summary, the outlined technique offers a systematic approach to synthesizing isoxazole derivatives, emphasizing their potential applications in medicine and materials research. These derivatives can be tailored through condensation, cycloaddition, and functionalization reactions to meet specific criteria, enabling the creation of molecules with desired properties. A comprehensive methodology covering material selection, purification, and structural analysis ensures the synthesis and validation of compounds with high quality. Evaluation metrics such as molar mass, quantity utilized, product yield, and quantity obtained provide valuable insights into reaction efficiency and success, guiding researchers in optimizing conditions for desired outcomes. Results indicate efficient synthesis of carboxamide and carbohydrazide derivatives, with carboxamide exhibiting superior performance in yield and product quantity. These findings underscore the importance of meticulous reaction design and optimization in chemical synthesis endeavors. This study advances the understanding and application of isoxazole chemistry, opening avenues for the development of innovative molecules tailored to various domains.The adaptability of isoxazole derivatives offers opportunities to address challenges in medicine development, materials design, and beyond, fostering innovation and

progress. Ongoing efforts will continue to explore and enhance synthesis processes, aiming to enhance the utility and effectiveness of isoxazole derivatives in meeting evolving industry requirements.

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