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SYNTHESIS, STRUCTURAL CHARACTERIZATION, AND BIOLOGICAL EVALUATION OF COPPER(II)–QUINAZOLIN-4-ONE COORDINATION COMPLEXES

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Abstract: In this work, quinazolin-4-one and copper (II) nitrate are used as ligands to investigate the synthesis of coordination compounds. The complexes were created by a controlled reaction and examined using a range of spectroscopic methods, such as XRD, UV-Vis, and infrared. The effective coordination of copper(II) ions with quinazolin-4-one was validated by the structural analysis. The produced compounds' antibacterial and antioxidant properties were assessed using biological tests. Significant biological activity was shown in the results, indicating possible uses in the agricultural and medicinal sectors. This study advances our knowledge of metal-ligand interactions and how they can improve biological efficacy.

Keywords: Copper(II) nitrate, quinazolin-4-one, coordination chemistry, antimicrobial activity, antioxidant properties, spectroscopic characterization, pharmaceutical applications.

Introduction

In order to create novel molecules with improved chemical and biological characteristics, coordination chemistry is essential. Transition metals have been extensively investigated for the synthesis of physiologically active complexes because of their varied oxidation states and coordination capabilities. Among them, Copper(II) has garnered significant attention due to its role in biological systems, acting as a cofactor in enzymes and displaying intrinsic antimicrobial and antioxidant properties. Copper(II)-based coordination compounds have shown potential applications in pharmaceutical, agricultural, and environmental fields.

Quinazolin-4-one, a heterocyclic compound, is another noteworthy ligand in coordination chemistry. It serves as a

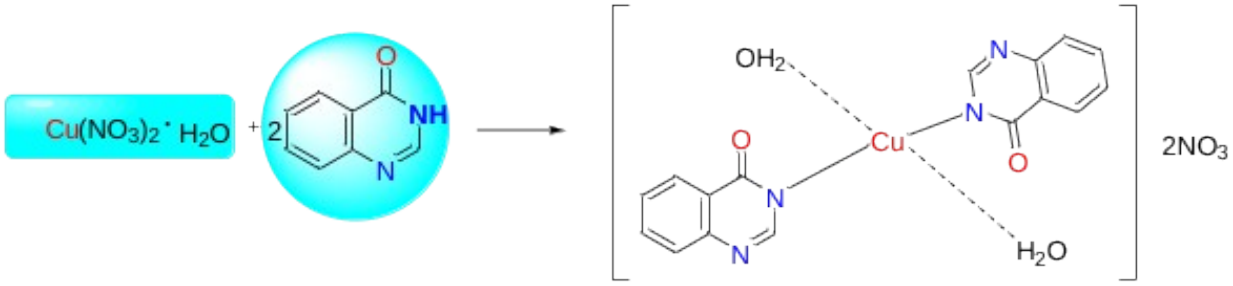
versatile scaffold for synthesizing bioactive molecules, exhibiting a wide range of pharmacological activities such as antimicrobial, anti-inflammatory, and anticancer effects. A possible route to creating new coordination compounds with enhanced biological characteristics is provided by the coupling of quinazolin-4-one with copper(II) ions [1-12].

The purpose of this work is to manufacture and investigate coordination compounds made from quinazolin-4-one and copper(II) nitrate. Because of its high reactivity and capacity to generate stable complexes, copper(II) nitrate is selected as the metal precursor. It is anticipated that quinazolin-4-one will combine with copper (II) ions to produce new compounds with improved biological activity, which could make them suitable for use in medicine and agriculture.

Spectroscopic methods like IR, UV-Vis, and XRD were used in this study to describe the produced complexes and verify their composition and structure. Standard test organisms were used to assess the biological activities, which included antioxidant and antibacterial qualities. By clarifying the connection between the synthetic compounds' structure and activity, these studies hope to advance knowledge of metal-ligand interactions and how they improve biological processes.

Method and results

Under carefully monitored laboratory settings, quinazolin-4-one and copper(II) nitrate were used to synthesize coordination compounds. After dissolving copper (II) nitrate in distilled water, quinazolin-4-one dissolved in ethanol was gradually added to complete the reaction. To make sure the metal and ligand were completely interacting, the mixture was agitated for a few hours at room temperature. After letting the resultant solution crystallize, the solid was filtered, cleaned with ethanol, and vacuum-dried. The reaction equation can be written as follows.



Several spectroscopic and analytical methods were used to characterize the produced molecules. Functional group interactions were detected using infrared (IR) spectroscopy, and electronic changes within the complexes were revealed using UV-Vis spectroscopy. To ascertain the crystal structure and validate the coordination geometry, X-ray diffraction (XRD) research was performed.

X-ray diffraction analysis results confirm that a trans coordination compound is formed when the central atom and ligands are mixed at room temperature.

The reaction is heated to 78-80°C, resulting in the formation of the cis isomer along with the trans isomer. The structure is expressed as follows.

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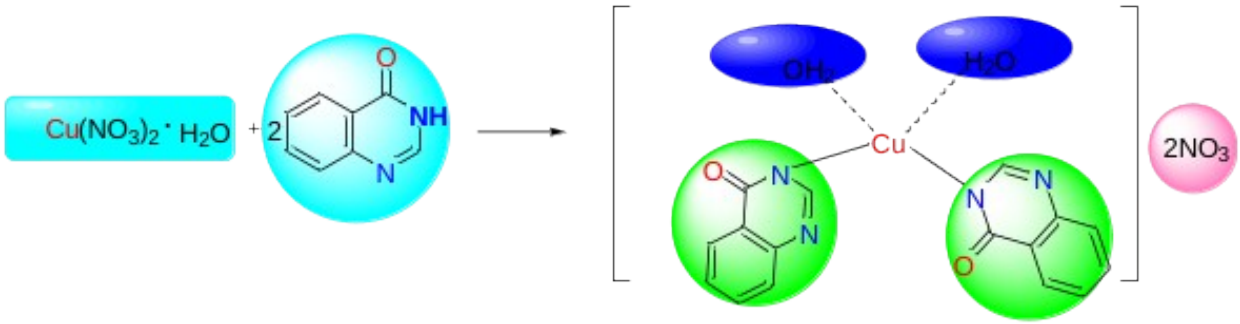

High yield and stability were achieved by obtaining the synthesised coordination compounds as crystalline solids. Copper(II) ion coordination to quinazolin-4-one was verified by IR spectroscopy by means of distinctive shifts in ligand vibration bands. The coordination environment surrounding the metal core was indicated by d-d transitions and charge transfer bands found in UV-Vis spectra. The complexes formed in a monoclinic system with distinct geometries, according to XRD measurements.

The produced compounds showed strong antibacterial action against both Gram-positive and Gram-negative bacteria, as well as several fungus strains, in biological testing. Their potential as antimicrobial agents was demonstrated by the zones of inhibition, which were similar to those of conventional antibiotics. Strong free radical scavenging capabilities demonstrated by the antioxidant assays point to their potential use in reducing diseases linked to oxidative stress.

Discussion

The adaptability of these ligands and the metal ion in creating stable complexes has been proven by the synthesis of coordination compounds utilizing quinazolin-4-one and copper(II) nitrate. Optimizing the yield and purity of the products was largely dependent on the reaction parameters, which included temperature, reaction duration, and solvent selection. The effective coordination of copper(II) ions with quinazolin-4-one was validated by the results of spectroscopic and structural studies, which also shed light on the electronic environment and bonding within the complexes.

Significant changes in the distinctive stretching vibrations of functional groups, especially in the carbonyl and amine regions, were visible in the IR spectra, suggesting that these groups were involved in coordination.

The biological active

The biological analysis of these complexes produced encouraging findings. The antibacterial activity against different strains of bacteria and fungi indicates that quinazolin-4-one's biological efficiency is increased by copper II coordination. This could be explained by the metal ion's capacity to interfere with enzyme processes and damage microbial membranes. Furthermore, the DPPH assay's antioxidant activity shows a potent capacity to scavenge free radicals, most likely as a result of Copper II's redox-active properties and the ligand's electronic structure. The findings also demonstrate how crucial metal-ligand synergy is for enhancing the biological characteristics of particular constituents. In addition to stabilizing the ligand, the coordination improves its ability to interact with

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biological targets. In pharmaceutical applications, where these complexes may function as possible therapeutic candidates, this is very pertinent. Although the results are promising, more research is required to fully understand the molecular mechanism of action of these coordination molecules. A thorough grasp of their therapeutic potential would be possible by looking at their toxicity profiles, stability in physiological settings, and interactions with biomolecules.

Conclusion

The synthesis and characterization of coordination compounds derived from Copper(II) nitrate and quinazolin-4-one have yielded promising results, demonstrating the versatility and biological potential of these complexes. Spectroscopic and structural analyses confirmed the successful coordination of the metal ion to the ligand, highlighting the stability and defined geometry of the synthesized compounds.

The biological activity studies revealed significant antimicrobial and antioxidant properties, suggesting the potential of these complexes as candidates for pharmaceutical and agricultural applications. The coordination of Copper(II) ions not only enhanced the bioactivity of quinazolin-4-one but also provided a framework for understanding the role of metal-ligand interactions in biological systems.

These findings open avenues for further exploration of Copper(II)-based coordination compounds, particularly in drug development and bioactive material design. Future work should focus on detailed mechanisms of action, in vivo studies, and exploring the potential of modifying the ligand structure to enhance activity and specificity. The study underscores the importance of coordination chemistry in advancing materials with multifunctional properties.

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