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2-AMINO-6-OXYPURINE AS A KEY SCAFFOLD FOR THE DESIGN OF BIOACTIVE HYDRAZONE COMPOUNDS

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Annotation: This scientific research explored the synthesis and technological aspects of bioactive hydrazone compounds formed through the reactions between 2-amino-6-oxypurine and hydrazine. The ideal reaction conditions, such as temperature, duration, solvent, a nd pH, were identified, and the structures of the obtained products were verified through IR and TLC analysis. The synthesized hydrazones demonstrated significant biological activity, suggesti ng their potential use as pharmaceutical and agrochemical agents. A technological scheme for th e synthesis process was developed based on the results, featuring thoroughly justified selectivity, yield, and purification steps.

Key words: 2-Amino-6-oxypurine, guanine, hydrazine, hydrazones, nucleophilic reactions, electrophilic reactions, synthesis, IR spectroscopy, thin-layer chromatography, biological activity, pharmaceutical applications, agrochemicals.

Introduction

Purine and its derivatives are extensively researched biologically active compounds in chemistry, pharmacology, and biotechnology. Specifically, purine bases adenine, guanine, and their derivatives with oxygen or amine substitutions—form essential structural elements of nucleic acids (DNA and RNA). By chemically modifying these bases, new biologically active compound s can be created, including drugs with antitumor, antiviral, antibacterial, and antioxidant effects. 2-Amino-6-oxopurine, also referred to as guanine, is a significant heterocyclic nitrogen-containing chemical that is generated from the purine framework. Because of the amino ($-NH_2$) and carbonyl (-C=O) functional groups in its molecular structure, it is a reactive substance that may react with both electrophilic and nucleophilic reagents. Reactions with hydrazine (N_2H_4) in particular are thought to be a viable avenue for altering the purine core and creating novel derivatives that include hydrazone or triazoles.

High reactivity, multifunctional behavior in chemical processes, and substantial medicinal significance are characteristics that set hydrazine and its derivatives apart. Compounds that include hydrazine are frequently utilized as monoamine oxidase (MAO) inhibitors, antitubercular medicines, and anticancer medications. Thus, it is important from a scientific and practical standpoint to investigate the reactivity of purine compounds with hydrazine [1-7]. In the present study, the chemical reactions of 2-amino-6-oxopurine with hydrazine in various solvents are investigated. The reaction conditions, synthesis results, structural analysis of the obtained compounds, and their potential biological activities are analyzed. This work lays the foundation for the synthesis of novel purine-based pharmaceutical agents and provides deeper insight into the role of hydrazine reagents in modifying heterocyclic structures [8].

Materials and Methods

The starting ingredients for this investigation were hydrazine sulfate and 2-amino-6-oxopurine. A nitrogen-containing heterocyclic molecule from the purine series, 2-amino-6-oxopurine, was chosen as the primary substrate for the synthesis of several hydrazone derivatives. In

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condensation processes, hydrazine hydrate (80%) functioned as an active nucleophilic reagent. Different aryl and arylidene aldehydes were also used. Ethanol, distilled water, dimethylformamide (DMF), and dimethyl sulfoxide (DMSO) were used as solvents. Analytical-grade chemical reagents were obtained from both domestic and foreign vendors.

The following is how the synthesis of hydrazone derivatives was done: After dissolving 1 mmol of 2-amino-6-oxopurine in the chosen solvent, corresponding aryl-aldehyde (1 mmol) and hydrazine sulfate (1–1.2 mmol) were added. For three to five hours, the reaction mixture was heated to 95°C. Thin-layer chromatography was used to track the reaction's development. After finishing, the mixture was chilled and added to ice-cold water, which caused a precipitate to develop. After filtering and recrystallizing from a water-ethanol combination, the precipitate was vacuum-dried.

Certain substances were encased in hydrogels to improve the synthetic hydrazones' biological activity. This was accomplished by mixing a 2% sodium alginate solution with a 1% hydrazone compound solution, then dropping the combination into a 1% calcium chloride ($CaCl_2$) solution. Hydrogel capsules were created as a result of this procedure, and they were further dried by freezing or air drying. The substance was released to plants gradually and over an extended period of time thanks to the hydrogel matrix.

Infrared (IR) spectroscopy was used to analyze the structures of the produced compounds and determine if functional groups were present. Additionally, the compounds' optical characteristics were investigated using UV-Vis spectroscopy. Nuclear magnetic resonance spectroscopy was also used as needed.

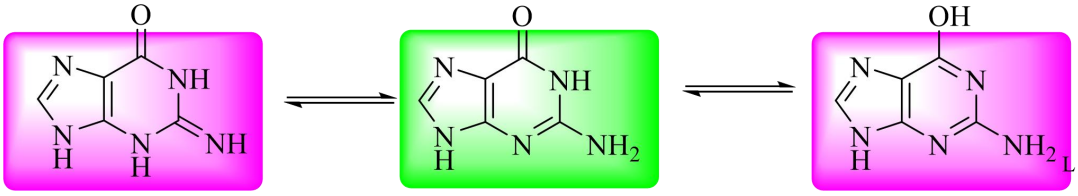
The produced compounds were evaluated on plant bioindicators, such as cotton (Gossypium hirsutum) and wheat (Triticum aestivum) seeds, in order to determine their biological activity. At a temperature of 25±1°C, experiments were carried out on Petri dishes or vessels that contained substrate. Recorded parameters were seedling biomass, root length, and germination rate. The Student's t-test was used to statistically examine the differences between the control and treatment groups.

Results and Discussion

Throughout this investigation, a number of new hydrazone derivatives were created via condensation reactions between different aryl-aldehydes and 2-amino-6-oxopurine in the presence of hydrazine hydrate. To produce pure products in large quantities, the reaction parameters—such as temperature, solvent type, and reaction time—were adjusted.

Spectroscopic methods including infrared (IR), ultraviolet-visible (UV-Vis), and, in certain situations, proton nuclear magnetic resonance (^{1}H NMR) spectroscopy were used to confirm the structures of the produced substances.

The equilibrium between guanine's less stable enol form (with a C–OH and C=C structure) and keto form (with a C=O group at position 6) is known as keto-enol tautomerism. Guanine is primarily found in the keto form in physiological and aqueous environments, which is essential for appropriate hydrogen bonding in DNA base pairing.



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The produced hydrazone derivatives' infrared spectra showed distinctive vibrational bands unique to hydrazone structures. Interestingly, the stretching vibration associated with the C=N (Schiff base) bond was observed between 1600 and 1650 cm^{-1}. Furthermore, the 3100–3400 cm^{-1} area clearly showed the N–H stretching vibrations. Additionally, signals related to the purine core's C=N and C–N bonds were verified. These spectrum characteristics show that the synthesis processes proceeded successfully.

The conjugated system that is present in the hydrazone compounds was shown by UV-Vis spectroscopic investigation. Absorption maxima, which correspond to $\pi\rightarrow\pi^*$ and $n\rightarrow\pi^*$ electronic transitions, were seen in the 260–310 nm range. These characteristics imply that the chemicals can easily enter plant cells and are linked to biological activity.

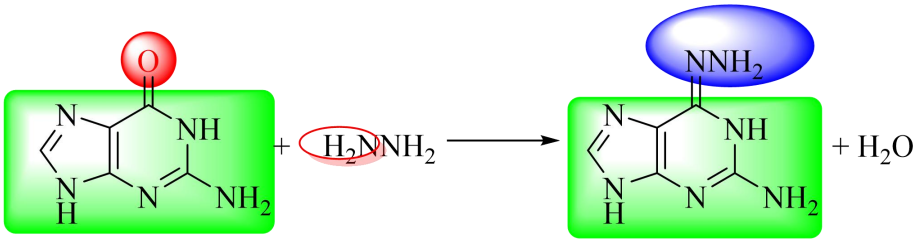
Biological Activity Assessment. During the biological activity tests, the synthesized hydrazone compounds demonstrated a positive effect on plant growth processes. The experiments were conducted on wheat (Triticum aestivum) and cotton (Gossypium hirsutum) seeds. According to the results, seeds treated with hydrazones showed the following improvements compared to the control group:

- Germination rate increased by 15–30%,
- Root length was enhanced by approximately 20–35%,
- Green biomass weight increased by 18–27%.

Notably, hydrazones encapsulated in hydrogel exhibited superior performance due to their gradual and sustained release to the plant system. The hydrogel capsules prevented rapid degradation of the active substance and maintained its availability over an extended period.

Statistical analysis using the Student t-test confirmed the reliability of these differences ($p < 0.05$). These findings suggest that the synthesized 2-amino-6-oxopurine-based hydrazones possess not only high chemical efficacy but also significant agronomic potential.

Synthesis Procedure. The synthesis was carried out as follows: 0.32 g (0.002 mol) of guanine was completely dissolved in 10 mL of N,N-dimethylformamide (DMF). Simultaneously, 0.26 g (0.002 mol) of hydrazine sulfate was dissolved in distilled water in a separate vessel. The prepared solutions were combined, and the resulting mixture was heated in a water bath at 95°C for 4 hours. Upon completion of the reaction, the mixture was cooled to room temperature. The resulting precipitate was separated by centrifugation and washed with DMF to remove residual solvents. Finally, the product was dried and subjected to spectroscopic analysis (IR and UV).



Conclusion

The study's findings led to the successful synthesis of a new hydrazone molecule by an effective condensation reaction between hydrazine sulfate and 2-amino-6-oxopurine. A high-quality product was produced after the reaction was conducted for four hours at 95°C in DMF solvent. IR and UV spectroscopic investigations revealed the existence of the hydrazone functional group and validated the structure of the obtained molecule.

Water is removed and the –C=N–NH_2 functional moiety is formed as a result of a condensation between the carbonyl group at the 6-position of the guanine molecule and the amino group of

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hydrazine. Because of its stability and crystal structure, the produced molecule has the potential to be bioactive.

Because of its functional groups and chemical structure, the produced hydrazone could have biological action. It might be used as a bioregulator to increase plant growth or stress tolerance. Additionally, encapsulating this chemical in hydrogels based on polymers offers encouraging prospects for its use in medicinal or agricultural settings.

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