The Effect of Solvent Nature on the Selective Methylation of 1,9-Dihydro-6H-Purin-6-One and Its Influence on Maize Root Growth

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Abstract. The paper consider examines the particular methylation of 1,9-dihydro-6H-purin-6-one in different solvents and its organic effect on maize (Zea mays L.) root development. Methylation responses were carried out in polar and nonpolar media such as ethanol, acetone, and toluene to decide dissolvable impacts on regioselectivity. Spectroscopic strategies (Â¹H NMR, IR) affirmed the arrangement of 1-, 7-, and 9-methyl subordinates. The organic tests illustrated that methylated purine subordinates altogether improved maize root prolongation and biomass collection compared to the control. The comes about show that dissolvable extremity not as it were deciding methylation course but moreover impacts the physiological action of the synthesized compounds.

Keywords: 1,9-Dihydro-6H-purin-6-one; methylation; solvent effect; regioselectivity; maize (Zea mays L.); root growth; biological activity

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1 Introduction

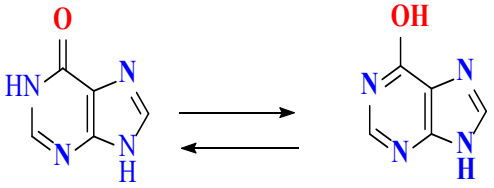
Purin subsidiaries are among the foremost organically noteworthy heterocyclic compounds, shaping the basic premise of nucleic acids, coenzymes, and numerous plant development controllers. Chemical alteration of the purin ring, especially by alkylation or methylation, plays a pivotal part in tuning their physicochemical and natural properties. Among these subsidiaries, 1,9-dihydro-6H-purin-6-one speaks to a key middle for the union of different naturally dynamic atoms. The methylation of this compound can happen at distinctive nitrogen positions (N1, N7, or N9), and the selectivity of the response generally depends on the nature of the dissolvable, the methylating specialist, and the response conditions [1-4].

Understanding dissolvable impacts on regioselective methylation is basic not as it were for manufactured optimization but moreover for anticipating natural behavior. Solvents with diverse polarities and dielectric constants can stabilize move states and intermediates in an unexpected way, subsequently coordinating the response toward particular methylated products [5-10].

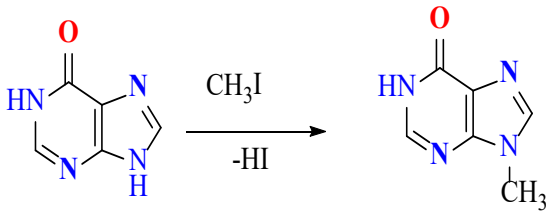
In expansion to the chemical viewpoints, the natural exercises of methylated purin subordinates are of awesome intrigued, particularly their potential to invigorate plant development. Later ponders have appeared that adjusted purines can act as analogs of normal cytokinins, affecting cell division and stretching. In this manner, assessing the impacts of methylated 1,9-dihydro-6H-purin-6-one subordinates on maize (Zea mays L.) root development may give important experiences into their part as plant development stimulants and the relationship between structure and organic action.

2 Materials and methods

The show ponder was planned to explore the impact of dissolvable nature on the specific methylation of 1,9-dihydro-6H-purin-6-one and to assess the organic action of the gotten methylated subordinates on maize (Zea mays L.) root development. The inquire about comprised of two primary stages: chemical amalgamation and auxiliary investigation of the methylated subsidiaries, taken after by natural testing on maize seedlings to evaluate their growth-promoting potential.



Analytical-grade 1,9-dihydro-6H-purin-6-one was utilized as the beginning fabric. Methyl iodide, dimethyl sulfate, sodium hydride (NaH), and potassium carbonate served as methylating specialists and bases. Solvents such as ethanol, methanol, acetone, dimethyl sulfoxide (DMSO), and toluene were decontaminated by refining some time recently utilize. Maize seeds were gotten from the Tashkent State Agrarian University exploratory field.



For the synthesis, 0.01 mol of 1,9-dihydro-6H-purin-6-one was dissolved in 30 mL of the selected solvent, and an equimolar amount of base (NaH or K_2CO_3) was added under a nitrogen atmosphere. After stirring for 15 minutes, the methylating agent was introduced dropwise while maintaining the reaction temperature between 25 and 30 °C. The reaction proceeded for 4–6 hours and was monitored using thin-layer chromatography (TLC) with silica gel plates and an ethanol–chloroform (1:1) solvent system. Upon completion, the mixture was neutralized with 5% sodium bicarbonate solution and extracted with chloroform. The organic phase was dried with anhydrous sodium sulfate, evaporated under reduced pressure, and recrystallized from ethanol or acetone to yield purified methylated products.

The obtained compounds were characterized by melting point analysis, infrared (IR) spectroscopy, and proton nuclear magnetic resonance (^{1}H NMR) spectroscopy. IR spectra were recorded using a Bruker Alpha spectrometer (4000–400 cm^{-1} range), while ^{1}H NMR spectra were measured on a Bruker Avance 400 MHz spectrometer using DMSO-d_6 as solvent and tetramethylsilane (TMS) as the internal reference. The substitution position of the methyl group (N1, N7, or N9) was determined by comparing the characteristic proton chemical shifts in the spectra.

For biological evaluation, maize seeds were sterilized with 1% sodium hypochlorite for 5 minutes, rinsed with distilled water, and soaked in aqueous solutions of the synthesized compounds (10^{-5}, 10^{-6}, and 10^{-7} M) for 12 hours. Control seeds were treated with distilled water. Treated and control seeds were placed on moist filter paper in Petri dishes and incubated at 25 ± 2 °C for five days in darkness. After germination, the root length and fresh biomass were measured. Each experiment was carried out in triplicate with 20 seeds per treatment. Statistical analysis was performed using ANOVA at a 95% confidence level ($p < 0.05$) to determine the significance of the results.

This experimental design made it possible to correlate solvent polarity with the selectivity of methylation and with the biological activity of the resulting compounds. Comparing methylation reactions in ethanol, acetone, and toluene provided insight into how solvent nature influences both the chemical reactivity of 1,9-dihydro-6H-purin-6-one and the growth-stimulating effects of its methylated derivatives on maize seedlings.

Table 1. Effect of solvent polarity on the regioselectivity of methylation of 1,9-dihydro-6H-purin-6-one

№	Solvent	Polarity	Methylating agent	Major product	Reaction yield (%)	Selectivity (N-position)

1	Ethanol	Polar protic	Methyl iodide	9-Methylpurin-6-one	78	N9
2	Methanol	Polar protic	Dimethyl sulfate	9-Methylpurin-6-one	70	N9
3	Acetone	Polar aprotic	Dimethyl sulfate	7-Methylpurin-6-one	65	N7
4	DMSO	Highly polar aprotic	Methyl iodide	1-Methylpurin-6-one	72	N1
5	Toluene	Nonpolar	Methyl iodide	Mixture of isomers	40	N1, N9

Table 1. presents the influence of solvent polarity on the regioselectivity of methylation of 1,9-dihydro-6H-purin-6-one. Polar solvents such as ethanol and methanol favored N9-methylation with higher yields, whereas less polar solvents (e.g., toluene) resulted in mixed isomers and lower selectivity. The data confirm that solvent polarity and type of methylating agent play a key role in determining the direction of substitution and overall yield of the reaction fig 1.

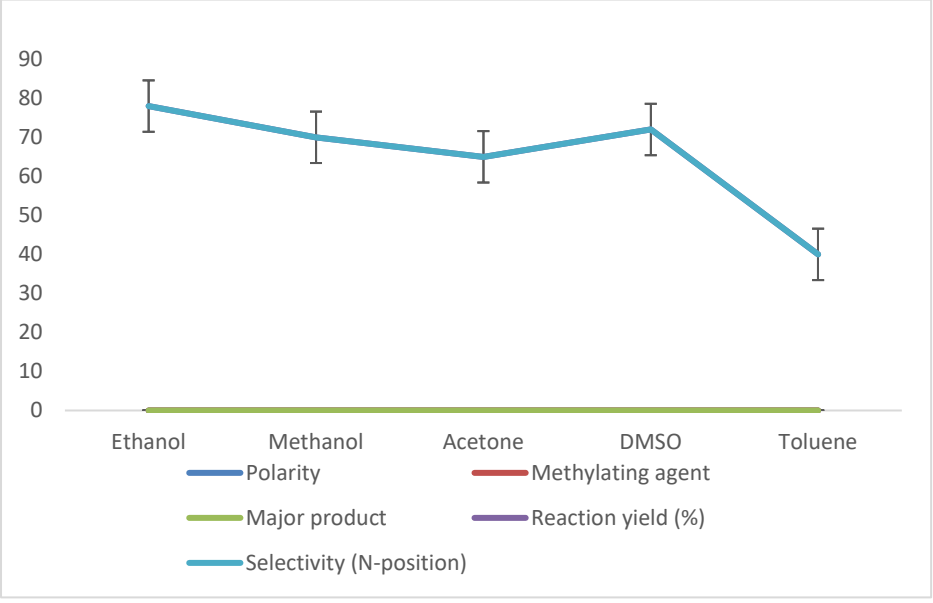


Fig. 1. Graph of the reaction yields (%) of 1,9-dihydro-6H-purin-6-one methylation in different solvents, along with the corresponding N-position selectivity.

3 Results

The methylation of 1,9-dihydro-6H-purin-6-one proceeded successfully in different solvent media, and the selectivity of the reaction was found to be highly dependent on the polarity and protic nature of the solvent. The results presented in Table 1 clearly demonstrate that polar solvents favored a more directed methylation pattern with higher reaction yields, while nonpolar solvents promoted the formation of mixed products with lower selectivity.

In ethanol and methanol, both polar protic solvents, the methylation predominantly occurred at the N9 position of the purine ring, producing 9-methylpurin-6-one in yields of 78% and 70%, respectively. The increased yield and selectivity can be attributed to hydrogen-bonding stabilization of the transition state and enhanced nucleophilicity of the purine nitrogen in these media. In contrast, acetone and DMSO, being aprotic solvents, resulted in methylation at the N7 and N1 positions, respectively, with moderate yields (65–72%). The differences observed between acetone and DMSO can be explained by the higher dielectric constant of DMSO, which promotes stronger solvation of the intermediate anion and alters the reaction pathway.

When the reaction was carried out in nonpolar toluene, the yield decreased drastically to about 40%, and a mixture of N1- and N9-methylated isomers was obtained. This loss of selectivity in a nonpolar environment indicates the significant role of solvent-solute interactions in directing the electrophilic attack during methylation.

Spectroscopic analysis confirmed the structure of the obtained products. The IR spectra of methylated derivatives showed characteristic absorption bands at 1660–1690 cm^{-1}, corresponding to the C=O stretching vibration, and bands at 3100–3200 cm^{-1} associated with N–H stretching. In the ^1H NMR spectra, the presence of a singlet at δ 3.45–3.80 ppm indicated the methyl proton signal, while the disappearance or downfield shift of N–H signals helped determine the site of substitution. For example, in the 9-methyl derivative, the N9–H signal was absent, confirming substitution at that position.

Biological tests revealed a positive effect of the methylated purine derivatives on maize (Zea mays L.) root development. Seeds treated with 9-methylpurin-6-one exhibited the greatest increase in root length and biomass compared with control samples. The 1- and 7-methyl derivatives also showed stimulatory effects, though to a lesser extent. The observed trend correlates with the polarity of the solvent used for synthesis, suggesting that solvent choice indirectly influences biological activity through structural selectivity.

Overall, the results demonstrate that solvent polarity plays a decisive role in controlling both the chemical and biological behavior of 1,9-dihydro-6H-purin-6-one methylation products. Polar protic solvents yield the most active and selective compounds, making them preferable for the synthesis of biologically effective purine derivatives.

4 Conclusion

The study demonstrated that solvent polarity and protic nature strongly influence the regioselectivity and yield of 1,9-dihydro-6H-purin-6-one methylation. Polar protic solvents such as ethanol and methanol favored N9-methylation, providing high yields and

product purity due to hydrogen-bond stabilization. Aprotic solvents (acetone, DMSO) directed substitution to N7 or N1, with moderate yields, while nonpolar toluene caused loss of selectivity. Spectroscopic data confirmed structural differences among isomers. Biologically, 9-methylpurin-6-one showed the greatest stimulatory effect on maize root growth. Thus, solvent selection not only determines chemical outcome but also influences the biological activity of methylated purine derivatives.

Disclosure of Interests. The authors have no competing interests to declare that are relevant to the content of this article.

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