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**RESEARCH ARTICLE**

# Synthesis of Triazol and Pyrimidyl Phenylurea: A New Plant Growth Regulator

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**Abstract:** Triazol and pyrimidyl phenylurea have been synthesized by the reaction of phenyl-isocyanate (**I**) with 3-amino-1,2,4- triazole (**II**) and 2-amino-4,6- dimethoxy pyrimidine (**III**). The product obtained triazol phenylurea (**IV**) and 4,6-dimethoxy pyrimidyl phenylurea (**V**) has plant growth regulator activity.

**Keywords:** Phenyl isocyanate, 3-Amino-1,2,4-triazole, 2- Amino-4,6-dimethoxypyrimidine reaction, Plant growth regulator activity

## Introduction

Urea and its derivatives constitute an important class of heterocyclic compounds which possess wide range agrochemical, therapeutic and pharmacological properties. Urea derivatives have been found to possess many promising biological activities such as herbicidal activity[1,3], antimicrobia[2], insecticides[4] and plant-growth regulators[5]. The modification of cyclic urea would have the potential to generate new functional molecules, which may result in interesting biological activities.

In this paper, we have reported the synthesis and characterization of triazol phenylurea and 4,6-dimethoxy pyrimidyl phenylurea. Compounds (IV and V) NMR, LCMS and IR analysis have been investigated to confirm the structure. The compound (IV) and (V) has plant growth regulator activity.

## Experimental

Phenyl isocyanate (Commercial) (**I**), acetonitrile (S d Fine), methanol (Commercial), activated charcoal (Sd Fine), 3-amino-1,2,4-triazole (E merck) (**II**) were used in the reaction.

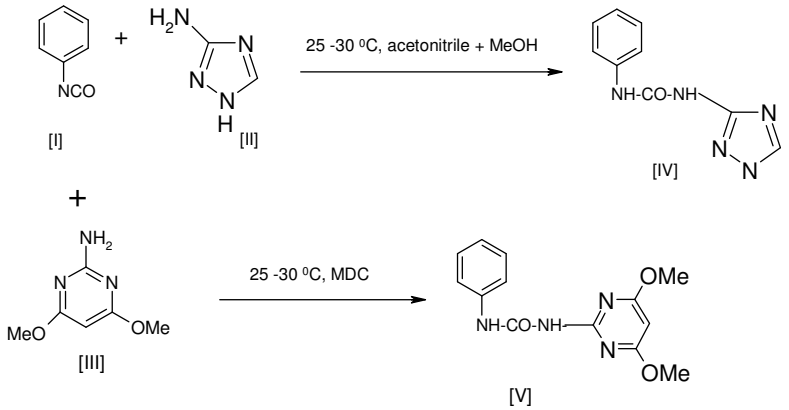
### *Method*

Acetonitrile 100 mL, 25 mL methanol and 3-amino-1,2,4- triazole 4.0 g ( 0.047 g mol) (**II**) was added to 250 mL round bottom flask (glass) fitted with mechanical stirrer and condenser

at room temperature. In the above reaction mass phenyl isocyanate 6.1 g (0.051 g-mol) was added over period 1.0 h by maintaining reaction mass temperature 25-30 $^{o}$C. Further reaction was maintained for 4 h at 25 to 30 $^{o}$C. Solvent was distilled under vacuum and residue was cooled to room temperature, the crude product (**IV**) was isolated by filtration and cake was washed with pet ether.

### *Purification*

The crude product was dissolved in 50 mL ethanol in hot condition. To this 0.01 g activated charcoal was added and stirred for 0.5 h and filtered through hyflow bed. The filtrate was cooled to 5 $^{o}$C and maintained the temperature for 5.0 h and then filtered. Product was dried under vacuum for 4 h at 50 $^{o}$C. Purity of the product (0.035 g-mole) was >97.0%, having over all yield is 74.5%.




**Scheme 1**

**Synthesis of compound 4,6 -dimethoxy pyrimidyl phenylurea (V)**

### *Materials*

phenyl isocyanate (Commercial) (**I**), methane dichloride(MDC) (Sd Fine), ethanol (Commercial), activated charcoal (Sd Fine), 2-amino-4,6-dimethoxy pyrimidine (Aldrich) (**III**) were used in the reaction.

### *Method*

Methane dichloride ( MDC) 50 mL, 2-amino-4,6-dimethoxy pyrimidine, 2.0 g ( 0.0128 g mol) (**III**) and was added to 100 mL round bottom flask (glass) fitted with mechanical stirrer and condenser at room temperature. To above reaction mass phenyl isocyanate 1.64 g (0.0138 g-mol) was added in 0.5 h by maintaining reaction mass at 25-30 $^{o}$C. Further reaction was maintained for 8 h at 25 to 30 $^{o}$C. MDC was distilled under vacuum and residue was cooled to room temperature and crude product (V) was isolated.

### *Purification*

The above crude product was dissolved in 25 mL ethyl acetate in hot condition. To this activated charcoal was added and stirred for 0. 5 h and filtered through hyflow bed. The filtrate was cooled to 0-5 $^{o}$C and maintained for 1.0 h and then filtered. Product was dried under vacuum for 3.0 h at 60 $^{o}$C. Purity of the product (0.0065 g-mole) was >97.0%, having over all yield is 50.8%.

## Results and Discussion

Triazol and pyrimidyl phenylurea have been synthesized according to the procedures given in the experimental section. The physical constants like melting point and solubility were determined for final product (**IV** and **V**). The compound was characterized by IR and $^1$H NMR and LCMS. The final product is solid off white color having melting point 164-166 $^o$C (**IV**) and 111-112 $^o$C (**V**) respectively.

*Spectral data of compound (**IV**)*

$C_9H_9ON_5$;NMR Data 6.47 ( s, 2H); 7.17- 7.20 ( m, 1H); 7.36-7.40 ( m, 2H); 7.53- 7.55 (m, 2H); 8.73 (s, 1H); IR Data (cm$^{-1}$) 3439 (-NH), 1644 (-C=O), 1502 (- CNH),1316 (- C-N) LCMS Data (m+1) → 203.8.

*Spectral data of compound (V)*

$C_{13}H_{14}O_3N_4$; NMR Data 3.97 (s, 6H); 5.74(s, 1H); 7.08-7.56 (m, 6H); 11.1 (s, 1H); IR Data (cm$^{-1}$) 3442 (-NH), 1686 (-C=O), 1580 (- CNH),1322 (-C-N) LCMS Data (m+1) → 274.8.

Plant growth regulator (PGR) activity of the above compounds has been studied for vegetable crop like lady finger in pot experiments (Table 1) by using 0.04% EC formulation.

**Table 1.** Growth and yield

| Compound | Average fruit growth in g | % Yield increase w.r.t. control |
|---|---|---|
| **IV** | 11.37 | 20.64 |
| **V** | 9.71 | 13.28 |

## Conclusion

Synthesis of the compound triazol phenylurea(IV) and 4,6 -dimethoxy pyrimidyl phenylurea (**V**) have been confirmed the structure by instrumental analysis: $^1$H NMR, FT-IR and LCMS. This product has unique combination of phenyl group and triazole ring as well as dimethyoxy substituted pyrimidine ring tested as plant growth regulator activity in different vegetable crop like lady finger. Both the compound has PGR effect.

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