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Synthesis of 2-Substituted 1,2,3-Triazoles of 3-Propargylquinazolone-4

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Abstract: This study is devoted to the synthesis of 1,2,3-triazoles derived from 3-propargylquinazolone-4. A convenient method has been developed for obtaining 2-substituted 1,2,3-triazoles of 3-(prop-2-ynyl)quinazolone-4. The article presents data on the influence of solvents on the yield of the final product.

Keywords: Quinazolone-4, propargyl bromide, 1,2,3-triazole, derivatives of 2-methylquinazolone-4, propargyl fragment, reaction center, yield.

Introduction. One of the promising directions in organic chemistry is the synthesis and study of heterocyclic compounds. These compounds find wide application in the synthesis of biostimulants for agriculture, pharmaceutical preparations, herbicides, fungicides, bactericidal and antifungal agents, special-purpose polymer materials, dyes, rubber stabilizers, and many others [1].

Molecules containing a propargyl group are unique due to the presence of two reactive centers: a triple carbon–carbon bond and a mobile terminal hydrogen. These centers enable addition, substitution, and cycloaddition reactions, leading to the formation of complex carbocyclic and heterocyclic compounds with high biological activity [2].

It is known that the cycloaddition reaction of phenyl azide to monosubstituted acetylenes yields two isomers: 1,4- and 1,5-isomers [3]. The ratio of these isomers depends on the nature of the substituent (e.g., aromatic or heterocyclic ring) in the acetylene group. However, reactions involving propyne derivatives bearing a quinazolone ring with phenyl azide have not been previously studied. It was of interest to investigate these interactions and determine the regularities of isomer formation.

The expected triazoles containing a quinazolone residue are of theoretical and practical interest in the search for biologically active compounds. Therefore, we investigated 2H-, 2-methyl-, and 2-phenyl-3-(prop-2-ynyl)quinazolones-4 in cycloaddition reactions. From the 1,3-dipolar cycloaddition of phenyl azide to 2-R-(prop-2-ynyl)quinazolones-4, we obtained 1-phenyl-4-(2-R-quinazolone-4-yl-3)-methyl-1,2,3-triazoles [4].

It is important to note that in these reactions, only the 1,4-isomer is formed, as confirmed by TLC analysis. This is explained by the electron-withdrawing effect of the quinazolone ring, which increases the polarizability of the triple bond and promotes the exclusive formation of the 1,4-isomer.

IR spectral analysis confirms the formation of the 1,4-substituted triazole heterocycle.

Physicochemical Constants and Spectral Characteristics of the Synthesized Triazoles

Compound No.	R Group	Yield (%)	m.p. (°C)	Molecular Formula	IR Spectra (cm^{-1})
IV	H	84	161–162	$C_{17}H_{14}ClN_5O$	1666 (C=O), 1612 (N=C), 1240 (–N₃), 1052/1034 (triazole ring)
V	CH_3	70	211–212	$C_{18}H_{16}ClN_5O$	1662, 1595, 1247, 1073/1042
VI	Ph	60	224–225	$C_{23}H_{18}ClN_5O$	1690, 1590, 1230, 1070/1050

These results confirm that the proposed structure of 1-phenyl-4-(2-substituted quinazolone-4-yl-3)-methyl-1,2,3-triazoles is correct. A simple and convenient method has been developed for the synthesis of these compounds.

A new heterocyclic system has been created that includes both a quinazolone and a 1,2,3-triazole ring, formed by 1,3-dipolar cycloaddition of phenyl azide to 2-H, 2-methyl, and 2-phenyl-3-(prop-2-ynyl)quinazolones-4.

Experimental Part. Synthesis of 1-phenyl-4-(2-R-quinazolone-4-yl-3)-methyl-1,2,3-triazole

Conclusion. To a solution of 1.84 g (0.01 mol) of 3-(prop-2-ynyl)quinazolone-4 in 20 mL of dry toluene, 1.31 g (0.011 mol) of freshly distilled phenyl azide was added. The reaction mixture was heated in a flask with a reflux condenser in an oil bath at 120–125°C for 6 hours.

After completion of the reaction, the solvent was evaporated, and the residue was recrystallized from acetone. The product was dried in a desiccator over fused $CaCl_2$. The yield was 2.15 g with a melting point of 175–176°C (yield: 71%).

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