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Syntheses and spectral elucidation of oxo pyrazolo Thiazolo pyrimidines

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Abstract
The syntheses of substituted 3-amino-4-oxo-2-N-(substituted) pyrazolo[3,4-*d*] thiazolo[3,2-*a*] pyrimidine was carried out by reaction of 6-cyano-5-oxo-7-(methylthio)-5*H*-thiazolo[3,2-*a*] pyrimidine with substituted hydrazino compounds in presence of weak base K_2CO_3 and N, N-dimethyl formamide as reaction solvent. The newly synthesized compounds were confirmed on the basis of Mass Spectroscopy, Infrared Spectroscopy and ^{1}HNMR Spectroscopy.

Keywords: 6-Cyano-5-oxo-7-(methylthio)-5*H*-thiazolo[3,2-*a*] pyrimidine, Hydrazine, K_2CO_3, N, N-dimethyl formamide

Introduction
The pyrazolo thiazolo pyrimidine heterocycles made up of three heterocyclic ring of pyrazole, thiazole and pyrimidine fusion. These fused heterocycles contain pharmacologically active Nitrogen and Sulpher containing pharmacophore. These structural fusion exhibit versatile chemical and biological properties to the resulting compounds, making them important scaffold for the development of new chemical drugs and bioactive molecules. The heterocyclic fused compounds containing thiazolo pyrazolo pyrimdine exhibit versatile biological activity [1, 2], antibacterial activity [3], anticancer activity [4], Xanthine oxidase activity [5], antimicrobial activity [6], anti-inflammatory activity [7], antitumor activity [8], insecticidal activity [9] and antiproliferative agent [10]. Based on the reported literature on the significance of thiazolo pyrazolo pyrimidines in medicinal chemistry field, chemist has sustained the attention of preparing thiazolo pyrazolo pyrimidine compounds.

In the present paper, we reported synthesis of substituted 3-amino-4-oxo-2-N-(substituted) pyrazolo[3,4-*d*] thiazolo[3,2-*a*] pyrimidine by condensing 6-Cyano-5-oxo-7-(methylthio)-5*H*-thiazolo[3,2-*a*] pyrimidine with selected nucleophile hydrazino compounds in N, N-dimethyl formamide (DMF) and anhydrous potassium carbonate. The synthesized compounds were characterized by IR, ^{1}HNMR and Mass spectroscopy. The present work provides significant method include simple, inexpensive experimental procedure, short reaction time, and good yield.

Experimental
All the chemicals used in present works are from analytical grade and used without further refinement. Melting points of the products were determined in open capillary tubes on an electro thermal melting point apparatus and were uncorrected. The development of reactions and the purity of the isolated compounds were monitored by thin layer chromatography (TLC) on Ultra Violet active silica gel plate (Merck). Infrared spectra were recorded on Shimadzu FT-IR spectrophotometer, ^{1}HNMR spectra were obtained on Bruker advance spectrophotometer 500 MHz in DMSO-d_6 using tetramethyl silane (TMS) as an internal standard. Mass spectrums were analyzed on GC-MS spectrometer using the electron spray ionization technique.

General Procedure
Synthesis of 3-amino-4-oxo-2-N-(substituted) pyrazolo [3,4-*d*] thiazolo [3,2-*a*] pyrimidine
A mixture of 6-cyano-5-oxo-7-(methylthio)-5*H*-thiazolo[3,2-*a*] pyrimidine (1) (0.223 g, 0.001 mol) and hydrazine hydrate and its different derivatives (2a-f) (0.001 mol) in 15 ml of N, N-dimethyl formamide as solvent and weak carbonate base anhydrous K_2CO_3 (10 mg) as catalyst was refluxed for 4-5 hours. The reaction mixture was cooled to room temperature and poured into ice cold water containing crushed ice. The separated solid mass of product was filtered, washed with ice cold water and recrystallized using absolute ethanol to give pure 3-amino-4-oxo-2-N-(substituted) pyrazolo [3,4-*d*] thiazolo [3,2-*a*] pyrimidine(3a-3f) (Scheme 1).

3-Amino-4-oxo-2-N-(*H*) pyrazolo [3,4-*d*] thiazolo[3,2-*a*] pyrimidine (3a)
Brown powder, Yield 81%, M.P.265°C (dec.). IR (KBr/cm^{-1}) 3430 (-NH_2 stretch), 3130 (-NH stretch), 1712 (>C=O stretch), ^{1}H NMR spectrum: (DMSO-d_6, δ ppm) 4.210-4.301 (s, 2H, -NH_2), 6.220-7.270 (m, 2H, thiazolic-H),9.110 (s,1H, -N-H), Mass spectrum: m/z 207 [M^+].

3-Amino-4-oxo-2-N-(phenyl) pyrazolo[3,4-*d*] thiazolo[3,2-*a*] pyrimidine (3b)
Brown powder, Yield 76%, M.P.281°C (dec.). IR (KBr/cm^{-1}) 3390 (-NH_2 stretch), 1716 (>C=O stretch), ^{1}H NMR spectrum: (DMSO-d_6, δ ppm) 3.970- 4.093 (s, 2H, -NH_2), 7.210-7.521 (m, 7H, -Ar-H & thiazolic-H), Mass spectrum: m/z 283[M^+].

3-Amino-4-oxo-2-N-(3'-methyl phenyl) pyrazolo [3,4-*d*] thiazolo [3,2-*a*] pyrimidine (3c)
Brown powder, Yield 78 %, M.P.278°C (dec.).IR (KBr/cm^{-1}) 3450 (-NH_2 stretch), 1733 (>C=O stretch), ^{1}H NMR spectrum: (DMSO-d_6, δ ppm) 2.582 (s, 3H, Ar-CH_3), 4.070-4.093 (s, 2H, -NH_2), 7.440-7.630 (m, 6H, -Ar-H & thiazolic-H), Mass spectrum: m/z 297 [M^+].

3-Amino-4-oxo-2-N-(4'-nitrophenyl) pyrazolo[3,4-*d*] thiazolo [3,2-*a*] pyrimidine (3d)
Brown powder, Yield 73%, M.P.270°C (dec.). IR (KBr/cm^{-1}) 3430 (-NH_2 stretch), 1715 (>C=O stretch), ^{1}H NMR

spectrum: (DMSO-d_6, δ ppm) 4.108- 4.268 (s, 2H, -NH_2), 7.210-7.598 (m, 6H, -Ar-H & thiazolic-H), Mass spectrum: m/z 328 [M^+].

3-Amino-4-oxo-2-N-(2',4'-dinitrophenyl) pyrazolo [3,4-*d*] thiazolo [3,2-*a*] pyrimidine (3e)

Brown powder, Yield 78%, M.P.288°C (dec.). IR (KBr/cm^{-1}) 3430 (-NH_2 stretch), 1722 (>C=O stretch), ^{1}H NMR spectrum: (DMSO-d_6, δ ppm) 3.890- 4.134 (s, 2H, -NH_2), 7.190-7.820 (m, 5H, -Ar-H & thiazolic-H), Mass spectrum: m/z 373 [M^+].

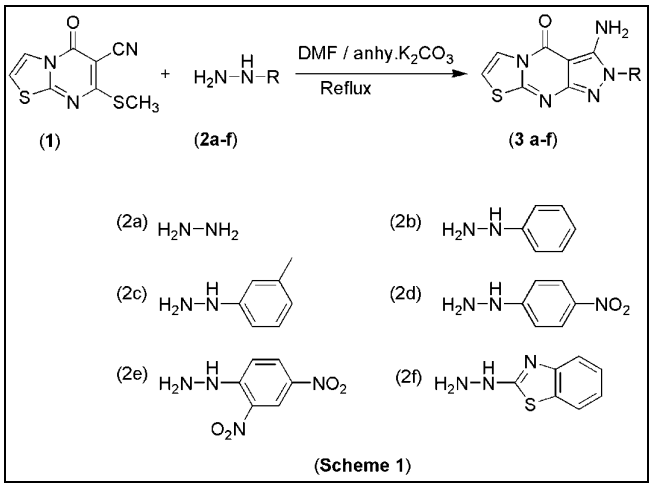
3-Amino-4-oxo-2-N-(2'-benzothiazolyl) pyrazolo[3,4-*d*] thiazolo [3,2-*a*] pyrimidine (3f)

Brown powder, Yield 79%, M.P.295°C (dec.). IR (KBr/cm^{-1}) 3470 (-NH_2 stretch), 1720 (>C=O stretch), ^{1}H NMR spectrum: (DMSO-d_6, δ ppm) 4.110- 4.245 (s, 2H, -NH_2), 6.550-7.760 (m, 6H, -Ar-H & thiazolic-H), Mass spectrum: m/z 340 [M^+].

Result and discussion

In present work, we reported suitable method for synthesis of 3-amino-4-imino-2-N-(substituted) pyrazolo[3,4-*d*] thiazolo [3,2-*a*] pyrimidine (3a-f) by reaction of 6-cyano-5-oxo-7-(methylthio)-5*H*-thiazolo[3,2-*a*] pyrimidine (1) and different hydrazino compounds using K_2CO_3 as catalyst and DMF as reaction solvent (Scheme 1). The yield of these synthesized compounds in the range of 73% to 81% with simple separation procedure. The structure of these synthesized compounds was confirmed on the basis of Mass, Infra Red and Proton Magnetic Resonance Spectroscopy.

6-cyano-5-oxo-7-(methylthio)-5*H*-thiazolo[3,2-*a*] pyrimidine (1) possess a replaceable active thiomethyl group at the 7-position which is activated electron withdrawing cyano group at 6-postion, which on reaction with selected substituted hydrazines independently in presence of catalytic amount (0.005 mol) of anhydrous potassium carbonate and N, N-dimethyl formamide as solvent with formation of (3a-3f).

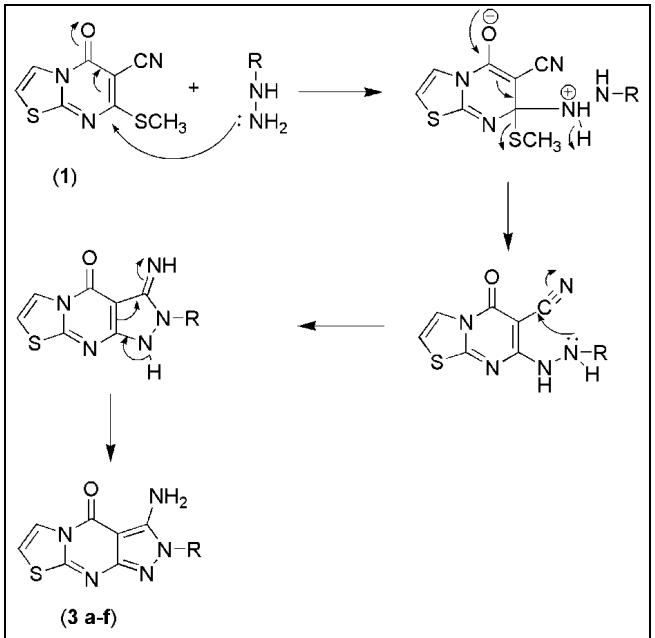


(Scheme 1)

Mass spectrum of synthesized compounds shows that molecular ion peak corresponds to molecular mass of respective compound which shows that formation of stable compounds 3a-f. Infrared spectra show absorption band in the range of 3470-3390 cm^{-1}, 1733-1712 cm^{-1} due to NH_2, >C=O stretching for compounds 3a–f respectively. The disappearance of absorption band at 2210 cm^{-1} indicates -CN group undergo cyclization to gain five membered pyrazole ring. Proton magnetic resonance spectral data also is in accord with structures assigned to compounds 3a-f.

^{1}HNMR spectra of these compounds showed absence of singlet at δ2.60 ppm due to thiomethyl protons indicates that cyclization took place. The new signals appears at δ3.89-4.33 ppm are due to -NH_2 proton.

The probable reaction mechanism for the formation of compound (3a-f) can be summarized as follows (Scheme 2).



(Scheme- 2)

Conclusion

Herein we have reported a convenient and efficient method for the synthesis of 3-amino-4-imino-2-N-(substituted) pyrazolo [3,4-*d*] thiazolo [3,2-*a*] pyrimidine by reaction of 6-cyano-5-oxo-7-(methylthio)-5*H*-thiazolo[3,2-*a*] pyrimidine and different hydrazino compounds using K_2CO_3 as catalyst and DMF as reaction solvent. This method provides diverse advantages, including the use of a reusable catalyst, affording high yields, employing a simple reaction procedure, and provides the simple isolation procedure. The synthesized compounds were confirmed on the basis of IR, ^{1}HNMR and Mass Spectroscopic analysis technique.

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