



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Synthesis and characterisations of some new 2,4-dihydro-[1,2,4]- triazol-3-one derivatives and X-ray crystal structures of 4-(3-phenylallylideneamino)-5-thiophen-2-yl-methyl-2,4-dihydro-[1,2,4] triazol-3-one

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Abstract: Compounds 2 were synthesised via the reaction of 4-amino-5-thiophen-2-yl-methyl-2,4-dihydro-[1,2,4]-triazol-3-one (1) with aldehydes. Compounds 3 and 4 were obtained from compounds 2 with bromo acetophenone and ethyl bromoacetate, respectively. The synthesis of compounds 2, 3, and 4 and crystal structure of compound 2a are being reported. The molecular structures were identified by IR, ¹H-NMR, ¹³C-NMR, MS, and elemental analyses. Compound 2a crystallises in the monoclinic P 2₁/n space group, with a = 6.565(5) Å, b = 18.278(5) Å, c = 13.8166(18) Å, β = 96.227(5)°, V = 1553.6(14) Å³, Z = 4. The newly compounds synthesised were screened for their antibacterial and antifungal properties. Among the compounds, 4d showed antimicrobial activity against *Candida albicans* ATCC 60193 and *Candida tropicalis* ATCC 13803.

Key Words: 1,2,4-Triazole, aldehydes, ethyl bromoacetate, bromo acetophenone, X-ray crystallography, antimicrobial activity

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