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Synthesis and characterization of novel triazol compounds containing a thiophen ring as potential antifungal agents and the structure of 2-(2-hydroxy-2-p-tolyethyl)-5-(thiophen-2-ylmethyl)- 4-(4H-1,2,4-triazol-4-yl)-2H-1,2,4-triazol-3(4H)-one

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Abstract: A series of new 4-(3,5-disubstitue-4H-1,2,4-triazol-4-yl)- 5-(thiophen-2-yl-methyl)-2H-1,2,4-triazol-3(4H)-ones (3a-c) were obtained by reaction N'-1-ethoxy-2-thiophen-2-yl-ethylydene hydrazino carboxylic acid ethyl ester (1) and 4-amino-4H-1,2,4-triazoles (2). 4-(3,5-disubstitue-4H-1,2,4-triazol-4-yl)-2-(2-oxo-2-arylethyl)-5- (thiophen-2-yl-methyl)-2H-1,2,4-triazol-3(4H)-ones (4a-e) and ethyl 2-(4-(3,5-disubstitue-4H-1,2,4-triazol-4-yl)-5-oxo-3-(thiophen-2-ylmethyl)- 4,5-dihydro-1,2,4-triazol-1-yl)acetates (6a-c) were obtained by reaction of compounds 3 and bromoacetophenon derivatives and bromo ethylacetate, respectively. Compounds 5a-e were synthesized from the reaction of corresponding compounds 4a-e with NaBH₄. Compounds 7a-c were obtained by the reaction compounds 6 and LiAlH₄.

Seventeen new compounds were synthesized and characterized by elemental analyses, IR, ¹H-NMR, and ¹³C-NMR spectral data. The structure of compound 5d was inferred through IR, ¹H-, ¹³C-NMR, elemental analyses, and X-ray spectral techniques. In addition, the newly synthesized chemicals were screened for their antibacterial and antifungal properties. Among the chemicals tested, 6a and 6b exhibited the highest degree of antifungal activity.

Key Words: Synthesis, 1,2,4-triazole-3-one, NaBH₄, LiAIH₄, antimicrobial activity, X-ray

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