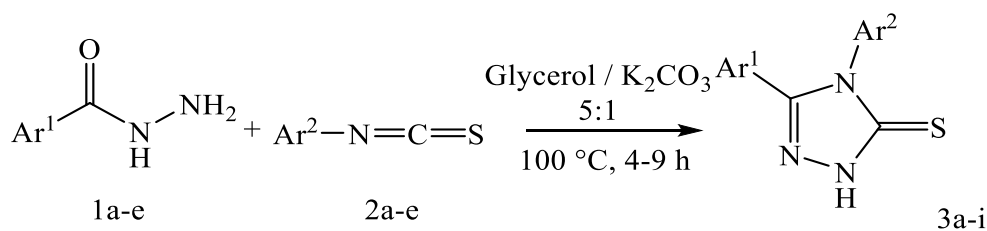


Abstract

Triazoles and their derivatives are important categories of heterocycles. These compounds are used in the synthesis of drugs. 1,2,4-triazoles contain medicinal properties such as antifungal, antiviral, antibacterial and antioxidant activities. In addition, the presence of sulfur atoms in the third position of 1,2,4-triazoles is necessary to increase the various biological activities of these compounds. These compounds can be present in two different forms of tautomerism that provide different reactivity. The results show that thion tautomers are of stable thiol tautomers. All tautomers thiol-thion reactions are exothermic and spontaneous. Entropy changes are negative during these tautomerization reactions. In the present work, the synthesis of some derivatives of 1,2,4-triazol-3-thione has been reported. The synthesized structures were confirmed by spectroscopic, IR and NMR data. In this research, a new and effective method in the presence of intense auxiliary solvents for the synthesis of new 1,2,4-triazole-3-thione derivatives from the reaction of phenyl hydrazid derivatives and phenyl isothiocyanates with a molar ratio of 1: 1 to be presented and Finally, anti-fungal, anti-bacterial and antioxidant activity of the derivatives was investigated. A mixture of potassium carbonate-glycerol was used as a Deep Eutectic solvent.



3a:Ar¹=C₆H₅, Ar²=4-O₂N-C₆H₄, 3b:Ar¹=4-HO-C₆H₄, Ar²=4-O₂N-C₆H₄, 3c:Ar¹=4-pyridin-C₆H₄, Ar²=4-O₂N-C₆H₄, 3d:Ar¹=4-furan-C₆H₄, Ar²=4-O₂N-C₆H₄, 3e:Ar¹=4-HO-C₆H₄, Ar²=4-O₂N-C₆H₄, 3f:Ar¹=4-O₂N-C₆H₄, Ar²=C₆H₅, 3g:Ar¹=4-O₂N-C₆H₄, Ar²=4-F-C₆H₄, 3h:Ar¹=4-O₂N-C₆H₄, Ar²=4-Me-C₆H₄, 3i:Ar¹=4-O₂N-C₆H₄, Ar²=4-Et-C₆H₄

Key words: Deep eutectic solvents, green chemistry, triazole, antifungal, antibacterial and antioxidant activities



University of Zabol

Graduate School

Faculty of Science

Department of Chemistry

The Thesis submitted for the Degree of Master of Science

(In the Field of Organic Chemistry)

Title:

one-pote Synthesis of 1,2,4-triazole-3-thione derivatives in deep eutectic solvent and evaluation of antibacterial and antifungal properties

First Supervisor:

Dr. Hamid Beyzaei

Secend Supervisor:

Dr. Reza Aryan

Advisor:

Dr. Noshin Mir

By:

Maryam Ghanbari kodeyani

Summer 2018