Regioselectivity of 1,3-dipolar cycloadditions and antimicrobial activity of isoxazoline, pyrrolo[3,4-d]isoxazole-4,6-diones, pyrazolo[3,4-d]pyridazines and pyrazolo[1,5-a]pyrimidines

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Abstract

Background: Isoxazoles exhibit interesting biological activities, and the 1,3-dipolar cycloaddition(13DC) reactions play an important role in both mechanistic and synthetic organic chemistry. Pyrazoles and annulated pyrazoles exhibit some diverse biological activities. They are used as antipyretic, analgesic drugs, tranquilizing, and herbicidal agents. Pyrazoles are also used extensively as useful synthons in organic synthesis. Pyrazolo[3,4-d]pyridazines showed good antimicrobial, anti-inflammatory and analgesic activities. Several oximes are found to be hyperglycemic, antineoplastic, anti-inflammatory, anti-leishmanial and VEGFR-2 kinase inhibitors.

Results: The present work describes an efficient synthesis protocol and molecular orbital calculations of isoxazoline and pyrrolo[3,4-d]isoxazole-4,6-dione derivatives from the reaction of hydroximoyl chloride with acrylonitrile, acrylamide, and N-arylmalemides. In addition, pyrazoles and pyrazolo[3,4-d]pyridazines are obtained via the reaction of 3-(dimethylamino)-1-(2,4-dimethyl-1,3-thiazol-5-yl)prop-2-ene-1-one with hydrazonoyl halides. Pyrazolo[1,5-a]pyrimidines were derived from condensation of either Sodium Salt of 3-Hydroxy-1-(2,4-dimethylthiazol-5-yl)prop-2-en-1-one (10) or 3-(dimethylamino)-1-(2,4-dimethyl)(1,3-thiazol-5-yl)prop-2-en-1-one (11) with aiminopyrozoles. A comparative study of the biological activity of the synthesized compounds with ampicillin and tetracycline is compiled in Table 3. Generally, all synthesized compounds showed an adequate inhibitory efficiency of growth of grampositive and gram-negative bacteria. Structures of the newly synthesized compounds were elucidated by elemental analysis, spectral data and a computational study.

Conclusions: In summary, new and efficient synthetic routes of isoxazoline, pyrrolo[3,4-d]isoxazole-4,6-dione derivatives, pyrazoles, pyrazolo[3,4-d]pyridazines and pyrazolo[1,5-a]pyrimidines have been achieved and the biological activity has been investigated.

Keywords

Author Keywords: Isoxazoline; Regioselectivity; 1,3-Dipolar cycloadditions; Density functional theory; Pyrrolo[3,4-d]isoxazole; Pyrazoles; Pyrazolo[3,4-d]pyridazines; Pyrazolo[1,5-a]pyrimidine

KeyWords Plus: DENSITY-FUNCTIONAL THERMOCHEMISTRY; HYDRAZONOYL HALIDES; EXACT-EXCHANGE; PYRAZOLE; DERIVATIVES

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