Available online at **www.joac.info**

ISSN: 2278-1862

Journal of Applicable Chemistry

2019, 8 (3): 1252-1263

(International Peer Reviewed Journal)

4*H*-Pyrimido[2,1-*b*]benzothiazole-3-Carboxamide Derivatives; Design, Synthesis, Biological Evaluation and Docking Studies

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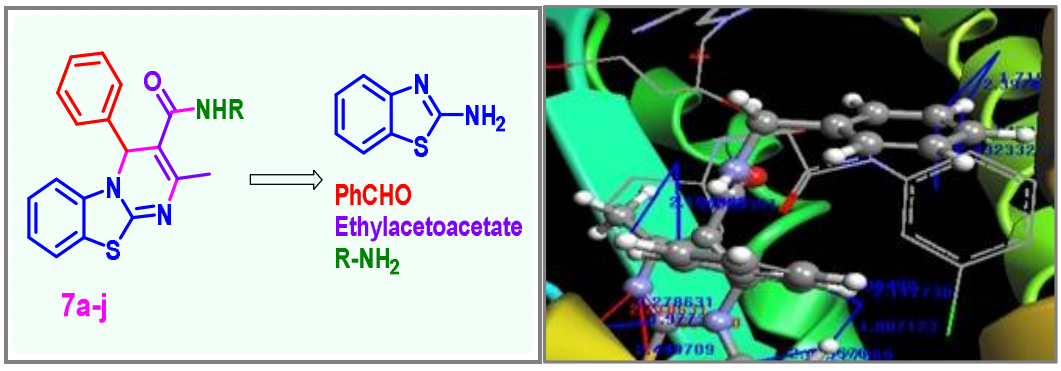
Accepted on 21st April, 2019

ABSTRACT

*Design and synthesis of a series of novel substituted 4H-Pyrimido[2,1-b]benzothiazole-3-carboxamides (**7a-j**) starting from commercially available and inexpensive starting materials (benzaldehyde, ethyl acetoacetate and 2-aminobenzothiazole) were generated and fully characterized using ^{1}H ^{13}C NMR, IR and mass spectral analysis. Furthermore, the synthesized compounds were tested for their in vitro antibacterial and antifungal activities, which indicated that the majority of 4H-Pyrimido[2,1-b]benzothiazole-3-carboxamides exhibit good to moderate activity compared to the standard drugs, streptomycin, penicillin and amphotericin-B. In particular, compounds **7b**, **7d**, **7j** have shown superior antibacterial activity against selected bacterial strains with 9.37μg mL^{-1}. Compound **7e** has shown excellent antifungal activity against A.niger with ZOI 48mm. The findings of biological activities are further supported by molecular docking studies. Experimental biological activities are exactly correlated with the docking scores.*

Graphical Abstract



Keywords: 2-Aminobenzothiazole, 4*H*-Pyrimido[2,1-*b*]benzothiazole, Molecular docking studies, Antimicrobial activity.