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Design, graph theoretical analysis, *in silico* modeling and synthesis of biologically active pyrimidines as antimicrobial and antitubercular agent

Theivendren Panneerselvam¹ and Jithendar Reddy Mandhadi²

¹Kalasalingam University, India

²Satavahana University, India

A series of 1-(2-(6-(4-substituted benzyl)-2-amino-5-carbamoylpyrimidin-4-yloxy)acetyl) thiosemicarbazide (S 1-25) 1-(2-(6-(4-substituted benzyl)-2-amino-5-carbamoyl pyrimidin-4-yloxy)acetyl) semicarbazide (R 1-25) were developed using different aromatic aldehydes, urea and thiourea. The synthesized compounds were characterized by IR, ¹H-NMR and mass spectrometry and these constitute attractive targets for the development of active antimicrobial as well as antimycobacterial agent. Among the compounds tested both electron withdrawing and releasing compounds exhibited significant antibacterial and antifungal activities while unsubstituted compounds also showed notable antifungal activity with reference to standard drugs Clotrimazole. The most active and selective compounds carry a fluorine atom in the phenyl ring at *para*-position. In conclusion, the potency and selectivity of these compounds make them valid lead compounds for synthesizing new analogues.

tpsphc@gmail.com