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Synthesis, Characterization, ADMET, Molecular docking and Pharmacological Evaluation of Some Novel Pyrimidine derivatives

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Abstract : Novel pyrimidine derivatives were synthesized by using urea or thiourea as a starting one. The synthesized derivatives were characterized by Infra-red, ^{1}H NMR, ^{13}C NMR, Ultraviolet, Mass spectrometry. Pharmacological appraisal of synthesised derivatives was done using agar diffusion method for antimicrobial and antifungal activity. The compound showed higher inhibition zones were further tested to determine their minimum inhibitory concentrations (MIC) utilizing serial dilution technique. The results showed the compound A_5 and A_8 have promising antimicrobial activity and compound A_5 have promising antifungal activity with MIC ranging from 11 to 20 ug/ml. Molecular docking studies were performed to inquisite binding pattern of the synthesised compound against antimicrobial peptide (PDB: 2L24) using Vlife MDS 4.6 version software. The synthesised compounds were analysed for their absorption, distribution, metabolism, excretion and toxicity properties. Results revealed the synthesised compounds have no ability to penetrate blood brain barrier, good bioavailability score and inactive immunotoxicity, cytotoxicity and aryl hydrocarbon receptor toxicity.

Keywords: Pyrimidine-5-carboxylate, antimicrobial, antifungal, molecular docking, ADMET.

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