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Synthesis, Molecular-Docking, and Biological Evaluation of Thiazolopyrimidine Carboxylates as Potential Antidiabetic and Antibacterial Agents

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Abstract : Heterocyclic compounds analogues and their derivatives have attracted strong interest in medicinal chemistry due to their biological and pharmacological properties. A series of new thiazolopyrimidine carboxylates were conveniently synthesized by one-pot three-component reaction of ethyl acetoacetate, 2-aminothiazole and benzaldehyde substituted with electron-donating and electron-withdrawing groups in order to find some more potent antidiabetic and antibacterial drugs. The structures of synthesized compounds were characterized by elemental analysis, IR, 1H NMR, 13C NMR spectroscopy. An in vitro antidiabetic effect was evaluated in adult male BALB/c mice and antibacterial activities were tested against Micrococcus luteus, Salmonella typhimurium, Bacillus subtilis, Bordetella bronchiseptica and Escherichia coli. Some of the tested compounds proved to possess good to excellent activities more than the reference drugs. An in silico molecular docking was also performed on synthesized compounds. The current study is expected to provide useful insights into the design of antidiabetic and antibacterial drugs and understanding the mechanism by which such drugs interact with RNA and diabetes target and exert their biochemical action.

Keywords : antidiabetic, antibacterial, MOE docking, thiazolopyrimidine
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