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Synthesis of thiophene-based flavone and pyrazole derivatives through intramolecular cyclization and condensation reactions: Molecular docking, biological evaluation including antimicrobial, antioxidant, and antitubercular activities

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ABSTRACT Synthesis of flavone derivatives was done by intramolecular cyclization of 1-(2-amino-2,4,5,6,7,7a-hexahydrobenzo[*b*]thiophen-3-yl)-3-substitued-phenylpropane-1,3-dione which was synthesized using the Gewald synthesis in the first step which is followed by Baker–Venkataraman rearrangement (BVR) reaction. Moreover, a series of pyrazole derivatives were synthesized through a condensation reaction between 1,3-diketone and hydrazine hydrate. The Fourier transform infrared (IR) spectroscopy, mass spectrometry (MS), and proton nuclear magnetic resonance results of the produced derivatives were validated. The biological potential such as the antimicrobial, antioxidant, and antimycobacterial activity of the produced compounds was evaluated. Antimicrobial screening outcomes showed that compound P_7 turned out to be the most effective antibacterial agent against *Staphylococcus aureus* (minimum inhibitory concentration [MIC] = 17.96 µM), *Bacillus subtilis* (MIC = 17.96 µM), *Escherichia coli* (MIC =9.34 µM), and *Salmonella typhi* (MIC = 17.96 µM); compound C_7 against *S. typhi* (MIC = 9.86 µM); and compound P_5 displayed remarkable antifungal activity toward each *C. albicans* and *A.niger* (MIC = 16.97 µM) with the standard drugs, cefadroxil (antibacterial), and fuconazole (antifungal). In comparison to ascorbic acid, a standard drug (IC_{50} = 44.91 µg/mL), compound C_{10} demonstrated good antioxidant activity, with an IC_{50} value of 41.84 µg/mL, according to the results of the antioxidant screening. With MIC values of 312.5 µg/mL and 625 µg/mL, respectively, compounds C_6 and C_{17} were shown to be efficacious in the *in vitro* anti-tuberculosis screening. A molecular docking study of an enzymatic active site of "*DprE1-decaprenylphosphoryl-ß-D-ribose-2'-epimerase*" shows a comparable binding mode to the native ligand with a good docking score which contributes to the understanding and development of models for ligand-protein interactions and create the fundamental structural framework for *Mycobacterium tuberculosis* inhibition.