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Synthesis, biological evaluation, and molecular docking of some new oxadiazole-incorporated pyrazole derivatives as potent antimicrobial agents

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ABSTRACT Our continuous effort in search of potent clubbed heterocycles and their newly designed derivatives, we have synthesized a series of some new of 1-(3,5-substituted diphenyl-4,5-dihydro-1-pyrazol-1-yl)-2-((5-phenyl-1,3,4-oxadiazol-2-yl)thio)ethan-1-ones (**5a–o**) by reacting 5-phenyl-1,3,4-oxadiazole-2-thiol (**4**) with 2-chloro-1-(3-(substituted phenyl)-5-substituted phenyl-4,5-dihydro-1*H*-pyrazol-1-yl)ethan-1-ones (**3a–o**). *In silico* molecular docking of new compounds has been demonstrated against 1BAG, 1JIJ, 1KZN, and 1Y54 using ciprofloxacin as a standard drug to ensure their potential. All compounds **5a–o** were subjected to antibacterial and antifungal biological evaluation. Antibacterial screening was carried out against two different Gram +ve strains *Staphylococcus aureus* and *Bacillus subtilis* as well as two Gram -ve strains, *Escherichia coli* and *Enterobacter aerogenes*. Antifungal activities were carried out against *Candida albican* and *Aspergillus niger*. Compound **5o** showed excellent inhibition values of 37, 23, 20, and 20 mm against *S. aureus, B. subtilis, E. coli,* and *E. aerogenes,* respectively, whereas compound **5e** exhibited good antibacterial activities against Gram-negative stains. We observed that compounds having electron-withdrawing groups are more effective against the Gram-positive strain, whereas compounds bearing electron-donating groups have displayed tremendous antifungal activities.

KEYWORDS Antibacterial, Antifungal, Molecular docking, Oxadiazole, Pyrazole.

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