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Synthesis, anti-bacterial evaluation, and molecular docking studies of some new aryl-piperazine tethered tetrazoles

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ABSTRACT Encouraged by the various pharmacological and biological importance of tetrazole hybrids in this work, we have synthesized some new 1-(4-(2-fluoro-4-(1*H*-tetrazol-1-yl)phenyl)piperazin-1-yl)ketone derivatives (6a-j) and evaluated them for *in vitro* antibacterial targets. The synthesis of target compounds **6a-j** was accomplished by the reaction of 1-(2-fluoro-4-(1*H*-tetrazol-1-yl)phenyl)piperazine **(4)** with various acyl chlorides. The synthesized compounds **6d, 6i,** and **6j** displayed noteworthy anti-bacterial activity. The tetrazole hybrid **6j** exhibited superior inhibition of *Enterobacter aerogenes* and *Bacillus subtilis* pathogens with MIC values of 111 ± 0.68 and 71 ± 1.92 µg/mL, respectively. The molecule **6c** was the most effective against *E. aerogenes*, *B. subtilis* with consecutive MIC's of 126 ± 0.88 µg/mL and 89 ± 1.74 µg/mL. Moreover, *in silico* molecular docking was performed to investigate the binding interactions between a series of target compounds (**6a-j**) and two key bacterial enzymes: DNA gyrase (PDB ID: 1KZN) and penicillin-binding protein **2a** (PBP2a, PDB ID: 5M18). In addition, to categorize the ligands accountable for the anti-bacterial activity, the mol dock simulations were performed with software AutoDock Vina 1.1.2. The obtained tetrazole hybrids **6j, 6f,** and **6c** gained superior binding energy values of −8.9, −8.7, and −8.1 kcal/mol with receptor 1KZN and −10.8, −10.1, and −9.9 kcal/mol with receptor 5M18. This work exemplifies numerous benefits of the molecular hybridization strategy to procure novel bioactive molecules. The obtained aryl-piperazine tethered tetrazole motifs were evaluated successfully for their antibacterial activities.

KEY WORDS Piperazine, Tetrazoles, Molecular hybridization, Antibacterial activity, Molecular docking.

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