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Design and synthesis of some new 1,2,4-triazole analogues as antimicrobial and anti-tubercular agents

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ABSTRACT Six new *N*-substituted 1,2,4-triazole derivatives, namely, 4-[4-(substituted phenyl)-5-sulfanyl-4*H*-1,2,4-triazol-3-yl]phenols, were synthesized from methyl paraben through the key intermediate 4-hydroxybenzohydrazide, followed by alkaline-mediated cyclization. The synthesized derivatives **(MA1-MA6)** were evaluated through *in silico* docking and absorption, distribution, metabolism, excretion, and toxicity (ADMET) predictions using PyRx and ADMETlab 2.0 to assess drug-likeness and receptor interactions. Among them, **MA1** and **MA2** exhibited the most potent antibacterial and antifungal activities, with minimum inhibitory concentration (MIC) values superior to ciprofloxacin and fluconazole. Both compounds also demonstrated strong activity against *Mycobacterium tuberculosis* H37Rv (MIC 0.125 µg/mL), comparable to standard drugs. Docking studies revealed strong binding interactions with microbial enzymatic targets, while ADMET analysis indicated favorable oral bioavailability and low toxicity. These findings highlight **MA1** and **MA2** as promising lead structures for the development of new antimicrobial and antitubercular agents.

KEY WORDS Anti-microbial activity, Anti-tubercular activity, 4-Hydroxybenzohyrazide, 1,2,4-Triazole.

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