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Synthesis and *in silico* studies of some new Schiff bases as antimicrobial and antitubercular agents

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ABSTRACT Ten pyridine carbohydrazide Schiff bases **(3a-3e)** and **(5a-5e)** were synthesized by refluxing pyridine carbohydrazides **1** and **4** with different ketones in the presence of ethanol and a few drops of glacial acetic acid. The synthesized compounds were biologically screened for antitubercular and antibacterial activity studies. The fit of these compounds within the active sites of the dihydrofolate reductase (DHFR) and enoyl ACP reductase was evaluated using molecular modeling techniques. The findings of the anticipated ADMET investigation showed that the compounds with the given names have drug-like characteristics. The newly synthesized molecules were subsequently tested for *in vitro* enoyl ACP reductase and DHFR enzyme inhibition, and molecules disclosed good inhibition values against enoyl ACP reductase and DHFR enzymes. The compounds **3b** and **5b** showed good antitubercular activity and antibacterial activity with 0.8 µg/mL along with promising InhA and DHFR enzyme inhibition evaluation.

KEYWORDS Carbohydrazide, Docking, Enzyme, Pyridine, Schiff base.

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