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Synthesis, *in silico* studies and antimicrobial activity of new pyrrolylbenzohydrazide Schiff bases

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ABSTRACT Two new series of pyrrolylbenzohydrazide Schiff bases **(3a-3e)** and **(5a-5j)** were prepared. Their suitability for the dihydrofolate reductase (DHFR) and enoyl acyl carrier protein (ACP) reductase active sites was evaluated using molecular modeling techniques. The results of the expected absorption, distribution, metabolism, excretion, and toxicity study demonstrated the drug-like properties of the pyrrolylbenzohydrazide Schiff bases. Following *in vitro* testing for enoyl ACP reductase and DHFR enzyme inhibition, some of the newly synthesized compounds exhibited good inhibition values against these enzymes. The results of *in vitro* anti-mycobacterial tests against the *Mycobacterium uberculosis* $H_{37}Rv$ strain revealed significant minimum inhibitory concentration values. Interestingly, compounds **3d**, **5c**, **5d**, **5e**, **5g**, and **5i** were shown to be active DHFR inhibitors with IC_{50} values of 32, 31, 32, 36, 32, and 30 μM, and active enoyl ACP reductase inhibitors with percent InhA inhibition values of 72, 78, 74, 77, 80, and 81 μM.

KEY WORDS Pyrrole, Schiff base, Dihydrofolate reductase enzyme, InhA enzyme, Molecular docking.

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