Indian Journal of Chemistry
Vol. 64, August 2025, pp. 815-822
DOI: 10.56042/ijc.v64i8.15813

Design, synthesis and evaluation of antitubercular activity of 4-oxo-butanamido benzoate derivatives

Sruthi Sri Bothsa, Sangeetha Guruvelli, Sony Priya Kurati, Patrick Francis Kimariyo & Murali Krishna Kumar Muthyala*

Pharmaceutical Chemistry Research Laboratory, AU College of Pharmaceutical Sciences,
Andhra University, Visakhapatnam 530 003, Andhra Pradesh, India

E-mail: profmmkau@gmail.com, dr.mmkkumar@andhrauniversity.edu.in

Received 26 December 2024; accepted (revised) 28 July 2025

In light of the inevitable emergence of resistance, designing small molecule-based new drug candidates through structure modulation of the reported drugs has garnered considerable attention. In present study, we have synthesized and characterized 4-oxo-butanamido benzoate derivatives as anti-TB agents through molecular hybridization. A total of 15 target compounds have been synthesized. Among all the tested compounds, three compounds (SA1a, SA1b and SA2a) show potent anti-TB activity with an MIC = 1.56 µg/mL against *M. tuberculosis* H37Rv. Further evaluation includes the testing for antibacterial and antifungal activities to assess selectivity. Testing has revealed neither antibacterial activity nor antifungal activity. Docking studies have been conducted to assess binding interactions of the synthesized compounds with the five key enzymes involved in the mycolic acid biosynthesis. Docking results reveal InhA as the potential enzyme target for these compounds. In present study, compounds SA1a, SA1b and SA2a show the highest binding affinity of below −10.0 KCal/mol. The overall conclusion has highlighted the activity potency to follow the pattern *para-* ≥ *meta-* > *ortho-* derivatives, with *para* derivatives exhibiting higher activity even in docking studies.

Keywords: *Mycobacterium tuberculosis*, 2-Transenoyl-acyl carrier protein (ACP) reductase (InhA), 4-Oxo-butanamido benzoate derivatives, MABA assay, Molecular docking