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Triazole-Diindolylmethane Conjugates as New Antitubercular Agents: Synthesis, Bioevaluation and Molecular Docking

Ashruba B. Danne[a], Amit S. Choudhari[b], Shakti Chakraborty[b], Dhiman Sarkar[b], Vijay M. Khedkar[c], Bapurao B. Shingate*[a]

[a]*Department of Chemistry, Dr. Babasaheb Ambedkar Marathwada University, Aurangabad 431 004, India*

[b]*Combi-Chem Bio-Resource Center, Organic Chemistry Division, CSIR-National Chemical Laboratory, Pune 411 008, India*

[c]*Department of Pharmaceutical Chemistry, Shri Vile Parle Kelavani Mandal's Institute of Pharmacy, Dhule, Maharashtra 424 001, India.*

E-mail: bapushingate@gmail.com (B. B. Shingate)*

**Corresponding author. Tel.: (91)-240-2403312; Fax: (91)-240-2403113*

Abstract

We have described the synthesis of novel triazole incorporated diindolylmethanes (DIMs) using molecular hybridization approach and their *in vitro* antitubercular activity against *Mycobacterium tuberculosis* H37Ra (ATCC 25177) both in active and dormant state. Among all the synthesized conjugates, the compounds **6b, 6f, 6l, 6n, 6q, 6r** and **6s** displayed good antitubercular activity against both active and dormant *Mtb* H37Ra strain. The compound **6l** exhibited good antitubercular activity against *Mtb* H37Ra dormant with IC_{50} value 1 µg/mL and IC_{90} (MIC) value 3 µg/mL. The compounds **6b, 6l** and **6r** displayed good antitubercular activity against *Mtb* H37Ra active with IC_{50} values 2.19, 1.52 and 0.22 µg/mL respectively. The compounds **6b, 6h, 6l** and **6s** displayed more than 70% inhibition towards *B. subtilus* strain against Gram-positive bacteria at 3µg/mL. The molecular docking study shows the binding modes of the titled compounds in active site of DprE1 enzyme and was helped to launch a structural basis for the inhibition of *Mycobacteria*.

Keywords: Antitubercular activity; Diindolylmethanes; 1,2,3-Triazoles; Molecular docking; Molecular hybridization

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Author affiliations

Abstract

We describe the synthesis of novel triazole-incorporated diindolylmethanes (DIMs) using a molecular hybridization approach. The *in vitro* antitubercular activity of the DIMs against *Mycobacterium tuberculosis* H37Ra (ATCC 25177) was tested in the active and dormant state. Among all the synthesized conjugates, the compounds **6b**, **6f**, **6l**, **6n**, **6q**, **6r**, and **6s** displayed

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