

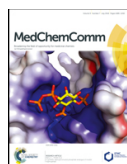


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Triazole–diindolylmethane conjugates as new antitubercular agents: synthesis, bioevaluation, and molecular docking †



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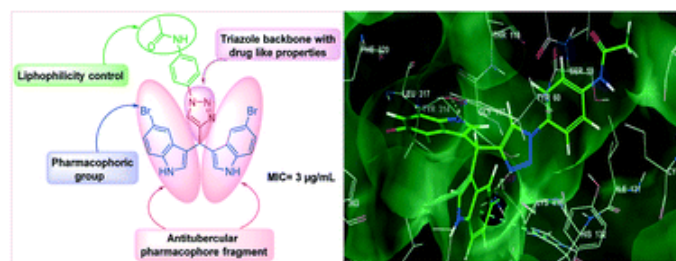
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Abstract

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 good antitubercular activity against both the active and dormant *Mtb* H37Ra strain. The compound **6l** exhibited good antitubercular activity against dormant *Mtb* H37Ra with an IC₅₀ value of 1 μg mL⁻¹ and IC₉₀ (MIC) value of 3 μg mL⁻¹. The compounds **6b**, **6l**, and **6r** displayed good antitubercular activity against active *Mtb* H37Ra with IC₅₀ values of 2.19, 1.52, and 0.22 μg mL⁻¹, respectively. The compounds **6b**, **6h**, **6l**, and **6s** displayed more than 70% inhibition against the Gram-positive *Bacillus subtilis* strain at 3 μg mL⁻¹. The molecular docking study showed the binding modes of the titled compounds in the active site of the DprE1 enzyme and assisted with elucidating a structural basis for the inhibition of *Mycobacteria*.

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