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Synthesis, computational docking, and biological evaluation of some new *N*-arylacetate nitroimidazole derivatives against *Mycobacterium tuberculosis*

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ABSTRACT This research aimed to design and synthesize innovative derivatives of 4-mono and 3,4-disubstituted aryl 4'-nitroimidazole acetates. The synthesis of these compounds involved a condensation reaction between 4-nitroimidazoles and 4-mono/3,4-disubstituted phenyl acetates. Their potential antitubercular properties were evaluated through *in vitro* and *in silico* methodologies. The results demonstrated potent anti-tubercular effects of these derivatives against *Mycobacterium tuberculosis*, particularly in the H37Rv strain, The observed activity is likely due to the role of the deazaflavin-dependent nitroreductase enzyme, which plays a crucial part in generating nitrous oxide radicals. The *in silico* studies aligned with the *in vitro* findings, highlighting that compound **NP-6** exhibited the most significant activity. Its effectiveness can be attributed to its capacity to establish strong hydrogen bonds, complemented by the role of the bromine atom as an electron-withdrawing group. These promising results suggest that further exploration of these compounds could lead to the development of effective anti-tubercular agents.

KEYWORDS Aryl acetates, Antitubercular activity, Docking, *Mycobacterium Tuberculosis*, Nitroimidazole

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