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Synthesis, biological evaluation, and molecular docking study of pyridine clubbed 1,3,4-oxadiazoles as potential antituberculars

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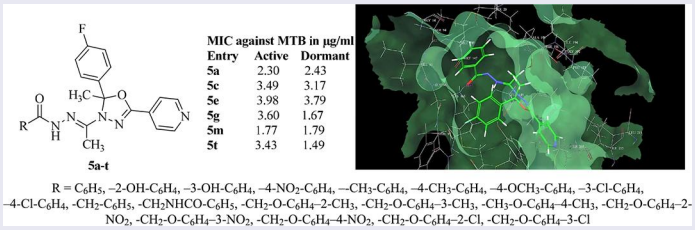
ABSTRACT

A series of pyridine clubbed 1,3,4-oxadiazole derivatives were efficiently synthesized, characterized by standard spectral techniques and evaluated for their *in vitro* antitubercular activity against *Mycobacterium tuberculosis* (MTB) $H_{37}Ra$ and *Mycobacterium bovis* BCG in active and dormant state using an established methods. Compounds **5a, 5m**, and **5t** were identified as the most active compounds against MTB. Molecular docking was performed against MTB enoyl-ACP (CoA) reductase (FabI/ENR/InhA) enzyme to predict the binding modes and affinity. The theoretical predictions from molecular docking could establish a link between the observed biological activity and the binding affinity shedding light into specific bonded and non-bonded interactions influencing the activity. The active compounds were studied for cytotoxicity against three cell lines and were found to be non-cytotoxic. Specificity of these compounds was checked by screening them for their antibacterial activity against four bacterial strains.

GRAPHICAL ABSTRACT



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KEYWORDS
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Introduction

Despite the availability of effective treatment regimens, tuberculosis (TB) remains a major global health problem being the second leading cause of death from infectious diseases

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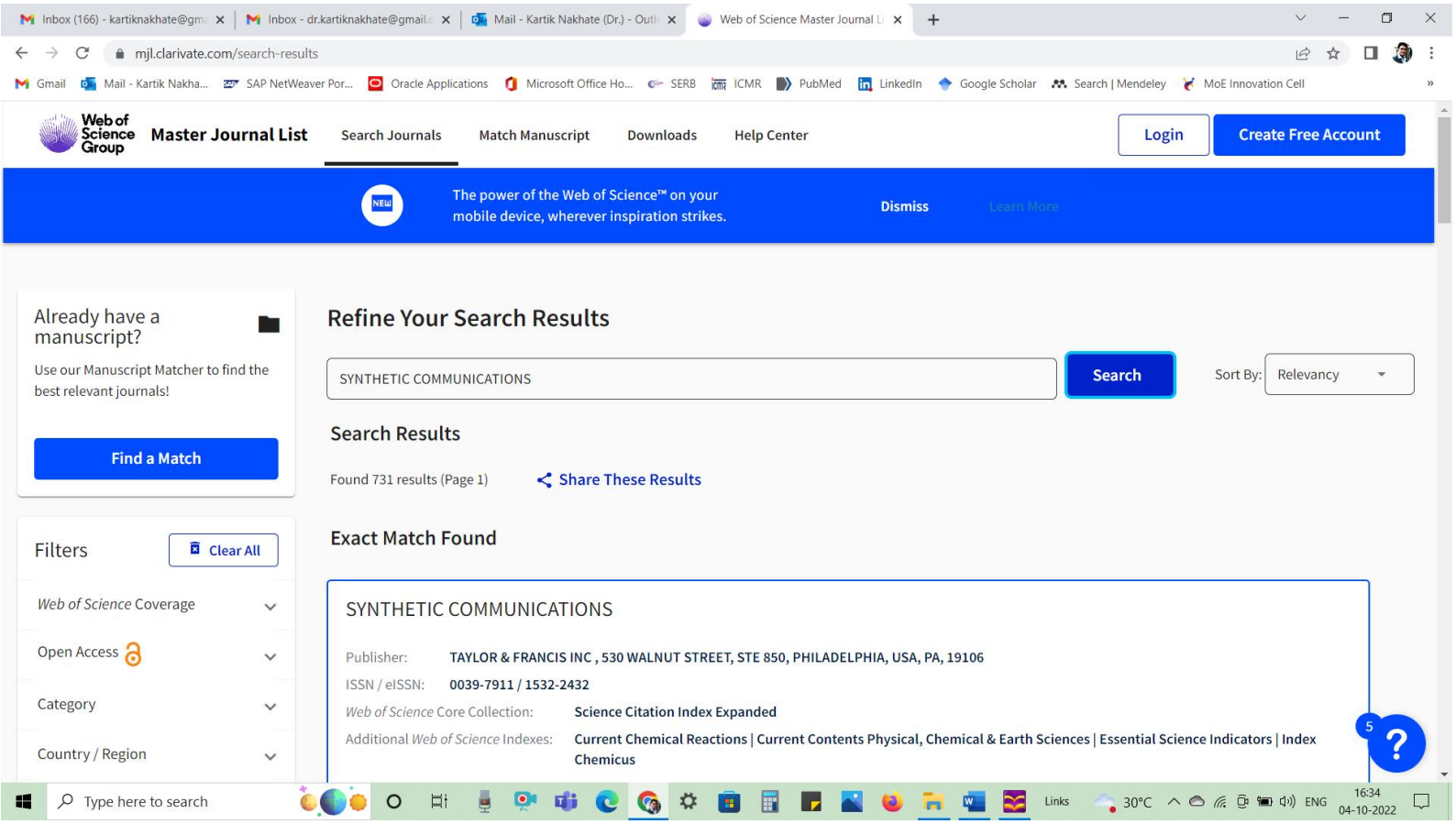
Supplemental data (full experimental detail, IR, ^1H and ^{13}C NMR, mass spectra and elemental analysis data) can be accessed on the publisher's website.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