





Design, synthesis and antitubercular assessment of 1, 2, 3-triazole incorporated thiazolylcarboxylate derivatives

Rajubai D. Bakale^a, Shubham M. Sulakhe^a, Sanghratna L. Kasare^a, Bhaurao P. Sathe^a, Sanket S. Rathod^b, Prafulla B. Choudhari^b, Estharla Madhu Rekha^c, Dharmarajan Sriram^c, Kishan P. Haval^a  

Show more 

 Share  Cite

<https://doi.org/10.1016/j.bmcl.2023.129551> 

[Get rights and content](#) 

Highlights

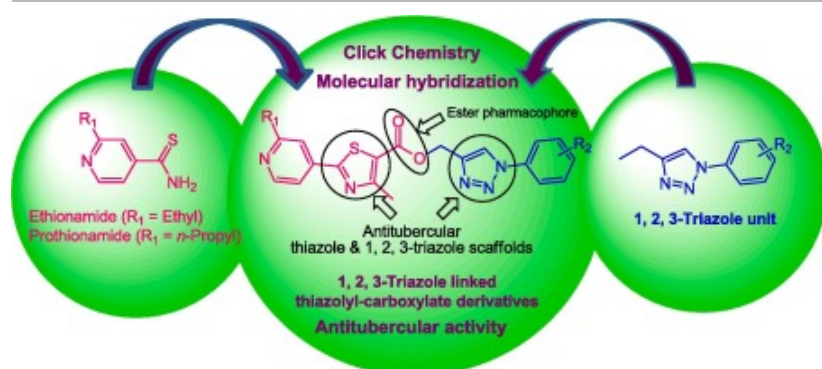
- A library of 1, 2, 3-triazole incorporated thiazolylcarboxylate derivatives was synthesized.
- The compounds were evaluated for their *in vitro* antitubercular activity against *Mycobacterium tuberculosis*.
- Two compounds were displayed potent antitubercular activity with MIC values of 1.56 and 3.12 µg/mL.
- Whereas, the four compounds were displayed noticeable antitubercular activity with a MIC value of 6.25 µg/mL.

Abstract

A library of 1, 2, 3-triazole incorporated thiazolylcarboxylate derivatives (**7a-q**) and (**8a-j**) were

synthesized and evaluated for their *in-vitro* antitubercular activity against *Mycobacterium tuberculosis* H37Rv. The two compounds **7h** and **8h** have displayed excellent antitubercular activity with MIC values of 3.12 and 1.56 $\mu\text{g}/\text{mL}$ respectively (MIC values of standard drugs; Ciprofloxacin 1.56 $\mu\text{g}/\text{mL}$ & Ethambutol 3.12 $\mu\text{g}/\text{mL}$). Whereas, the four compounds **7i**, **7n**, **7p** and **8i** displayed noticeable antitubercular activity with a MIC value of 6.25 $\mu\text{g}/\text{mL}$. The active compounds of the series were further studied for their cytotoxicity against RAW264.7 cell line using MTT assay. Furthermore, to study the probable mechanism of antitubercular action, physicochemical property profiling, DFT calculation and molecular docking study were executed on mycobacterial cell wall target *Decaprenylphosphoryl- β -D-ribose 2'-epimerase 1* (DprE1). Among all the compounds, **7h** (-10 kcal/mol) and **8h** (-10.1 kcal/mol) exerted the highest negative binding affinity against the targeted DprE1 (PDB: 4NCR) protein.

Graphical abstract



Download : [Download high-res image \(279KB\)](#)

Download : [Download full-size image](#)

Section snippets

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper...

Acknowledgement

We thank Dr. Babasaheb Ambedkar Marathwada University, Aurangabad for financial assistance (MRP File No. Plan&Stat/RDC/2022-23/732-36). RDB is thankful to SARTHI for financial assistance in the form of the Chhatrapati Shahu Maharaj National Research Fellowship...

[Recommended articles](#)

References (81)

J.A. Garrido-Cardenas *et al.*

Tuberculosis (2020)

V. Singh *et al.*

Drug Discov Today (2017)

Y. Sajja *et al.*

Bioorg Med Chem Lett (2017)

R. Majeed *et al.*

Eur J Med Chem (2013)

M.B. Muluk *et al.*

J Heterocycl Chem (2019)

R. Paprocka *et al.*

Bioorg Med Chem Lett (2015)

M.H. Shaikh *et al.*

Bioorg Med Chem Lett (2016)

G. Wang *et al.*

Bioorg Med Chem Lett (2016)

D. Dheer *et al.*

Bioorg Chem (2017)

D. Kumar *et al.*

Eur J Med Chem (2014)



[View more references](#)

Cited by (5)

Novel sulphonamide-azaheterocycle conjugates and their anti-cancer, anti-inflammatory, anti-diabetic, anti-angiogenesis activity and molecular docking studies

2024, Results in Chemistry

Show abstract 

Synthesis, Characterization, In Silico DFT, Molecular Docking, and Dynamics Simulation Studies of Phenylhydrazono Phenoxyquinolones for Their Hypoglycemic Efficacy

2024, ACS Omega

Synthesis and in vitro evaluation of tetrahydropyridines as potential CDK2 and DprE1 inhibitors

2024, Research on Chemical Intermediates

Synthesis and In Vitro Antitumor Activity Evaluation of Gefitinib-1,2,3-Triazole Derivatives

2024, Molecules

High-throughput computational screening for identification of potential hits against bacterial Acriflavine resistance protein B (AcrB) efflux pump

2024, Journal of Biomolecular Structure and Dynamics

View full text

© 2023 Elsevier Ltd. All rights reserved.



All content on this site: Copyright © 2024 Elsevier B.V., its licensors, and contributors. All rights are reserved, including those for text and data mining, AI training, and similar technologies. For all open access content, the Creative Commons licensing terms apply.

