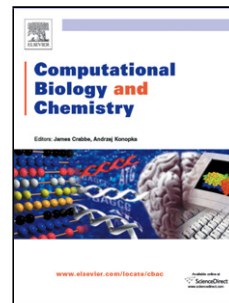


Accepted Manuscript

Title: Synthesis, antibacterial activity, synergistic effect, cytotoxicity, docking and molecular dynamics of benzimidazole analogues

Authors: Ritika Srivastava, Sunil K. Gupta, Farha Naaz, Anuradha Singh, Vishal K. Singh, Rajesh Verma, Nidhi Singh, Ramendra K. Singh



PII: S1476-9271(18)30248-2
DOI: <https://doi.org/10.1016/j.compbiolchem.2018.05.021>
Reference: CBAC 6871

To appear in: *Computational Biology and Chemistry*

Received date: 8-4-2018
Revised date: 18-5-2018
Accepted date: 24-5-2018

Please cite this article as: Srivastava, Ritika, Gupta, Sunil K., Naaz, Farha, Singh, Anuradha, Singh, Vishal K., Verma, Rajesh, Singh, Nidhi, Singh, Ramendra K., Synthesis, antibacterial activity, synergistic effect, cytotoxicity, docking and molecular dynamics of benzimidazole analogues. *Computational Biology and Chemistry* <https://doi.org/10.1016/j.compbiolchem.2018.05.021>

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

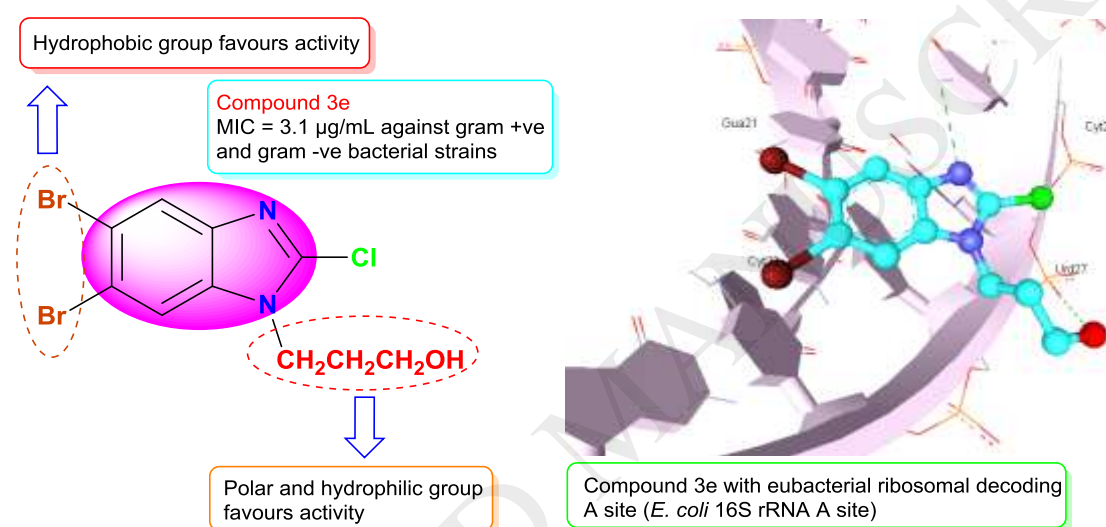
Synthesis, antibacterial activity, synergistic effect, cytotoxicity, docking and molecular dynamics of benzimidazole analogues

Ritika Srivastava^a, Sunil K. Gupta^a, Farha Naaz^a, Anuradha Singh^a, Vishal K. Singh^a, Rajesh Verma^a, Nidhi Singh^a and Ramendra K. Singh^{a*}

^aBioorganic Research Laboratory, Department of Chemistry, University of Allahabad, Allahabad-211002, India

*Corresponding author: Ramendra K. Singh, rksinghsrk@gmail.com

Graphical abstract



Highlights

- New benzimidazole analogues were synthesized as potential antibacterial agents.
- The molecules were docked with eubacterial ribosomal decoding A site (*E. coli* 16S rRNA A site).
- Fractional inhibitory concentration (FIC) was determined using combination approach showed synergistic effect.
- Molecular Dynamics simulation studies were indicated about stable ligand-protein complexes.
- Cytotoxicity assay against PBM, Vero and CEM cell lines proved that the active analogues were less cytotoxic than the reference drugs used.

Download English Version:

<https://daneshyari.com/en/article/6486785>

Download Persian Version:

<https://daneshyari.com/article/6486785>

[Daneshyari.com](https://daneshyari.com)