Indian Journal of Heterocyclic Chemistry
Vol. 35 - Number 03 (Jul-Sep 2025) 673-680
https://connectjournals.com/01951.2025.35.673
https://doi.org/10.59467/IJHC.2025.35.673

ISSN (Print) : 0971-1627
ISSN (Online) : 2456-4311

Biaryl piperidine derivatives: Synthesis, antileishmanial efficacy, and molecular docking studies

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ABSTRACT A series of biaryl piperidine derivatives **6-14** was synthesized and evaluated for antileishmanial efficacy against the *Leishmania donovani* strain Ag83. The Suzuki reaction of the bromo compound yielded biaryl compounds **6-8**. Boc protection of **6-8** resulted in the formation of piperidine derivatives as hydrochloride salts (**9-11**), and subsequent ester hydrolysis gave pure biaryl amino acid derivatives (**12-14**). The target compounds **8-11** and **13** showed promising antileishmanial activity. The hydrochloride salts of biaryl piperidines, **9** and **10** exhibited the 60.2% and 57.2% inhibition respectively at 20 μM concentration and further inhibited the proliferation by 63.7%, 64.0%, 64.7%, 64.8%, 69.2%, and 64.6, 64.8%, 64.8%, 66.4%, 67.9%, respectively, at 40, 80, 100, 150, and 300 μM concentrations. The respective IC_{50} values for compounds 9 and 10 are 16 μM and 17 μM. The compounds chosen for this study were additionally analyzed through molecular docking, and the binding affinities correspond with the biological findings. The emergence of these new compounds will enable the development of new drugs for targeting Leishmaniasis.

KEY WORDS Antileishmanial activity, Promastigotes, Biaryl Piperidines, Leishmanolysin, Neglected tropical diseases.

How to cite this article: Narsaiah, C., Rathnakar, B., Nimma, R., Goud, S.S.K., Sinha, K.K., Prasad, S.R. and Satyanarayana, M. Biaryl piperidine derivatives: Synthesis, antileishmanial efficacy, and molecular docking studies, *Indian J. Heterocycl. Chem.*, **2025**, *35*, 673–680. *https://doi.org/10.59467/IJHC.2025.35.673*