Indian Journal of Heterocyclic Chemistry
Vol. 31 - Number 03 (Jul-Sep 2021) 423-433
DocID: https://connectjournals.com/01951.2021.31.423

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

Development of Imidazoline-2-one Derivatives as Potential Antifungal and Anthelminthic Agents: *in silico* and *in vitro* Evaluation

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ABSTRACT Based on appropriate values of synthetic accessibility concerning from ADMET properties and docking scores by docking against proteins 3OZU and 1OJ0, a series of 4,5-diphenyl-1*H*-imidazol-2-ones ($\mathbf{I}_{1\text{-}15}$) were synthesized. The key intermediate, 2-hydroxy-1,2-disubstitutedethanones ($\mathbf{E}_{1\text{-}15}$) were prepared by benzoin condensation using 2:1 ratio of aromatic aldehydes and thiamine in the presence of alkali. Further, these cyclized ethanones ($\mathbf{E}_{1\text{-}15}$) were treated with urea to yield 4,5-diphenyl-1*H*-imidazol-2-one derivatives ($\mathbf{I}_{1\text{-}15}$) and were characterized by IR,^{1}H NMR, Mass spectra, and CHNO analysis. The synthesized compounds were screened for their anthelmintic potential on *Pheretima Posthuma* along with standard albendazole, and antifungal activity (minimum inhibitory concentration method) on *Candida albicans* and *Aspergillus niger* along with standard miconazole. The results revealed that among all the tested compounds $\mathbf{I}_3$, $\mathbf{I}_4$, and $\mathbf{I}_7$ show considerable synthetic accessibility, docking scores, anthelminthic, and antifungal activity.

KEYWORDS Molecular docking, ADMET studies, Imidazol-2-ones, Anthelmintic activity, Antifungal activity.

How to cite this article: Mallela, V.J., Chilamakuru, N.B., Shaik, S.B., Simham, V., Peraman, R., Singirisetty, T. Development of Imidazoline-2-one Derivatives as Potential Antifungal and Anthelminthic Agents: *in silico* and *in vitro* Evaluation, *Indian J. Heterocycl. Chem.,* **2021**, *31*, 423–433. *(DocID: https://connectjournals.com/01951.2021.31.423)*