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Área: MED

Identification of a Novel Antileishmanial Compound Through Combined In Vitro and In Silico Approaches

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Visceral leishmaniasis; Drug Discovery; Pharmacokinetics.

Highlights

In vitro identification of a novel antileishmanial compound. Study of cell cycle using flow cytometry. Characterization of target using DFT and molecular docking. Pharmacokinetics evaluation using in vitro approach.

Resumo/Abstract

Leishmaniasis comprises a group of diseases caused by intracellular protozoa of the genus *Leishmania*. Among the different forms of leishmaniasis, visceral leishmaniasis (VL) is the most severe and can be fatal if left untreated. In this study (**Figure 1**), a series of compounds were evaluated against the intracellular form of *Leishmania*, leading to the identification of a promising candidate (IC_{50} = 0.49 µM and CC_{50} > 64µM). Flow cytometry assays revealed that this compound modulates the parasite's cell cycle, possibly inducing arrest in the G0/G1 phase, a critical stage for parasite growth and protein synthesis. Since proper cell cycle progression is essential for *Leishmania* proliferation and survival, this disruption may contribute to its antiparasitic activity. Computational studies using DFT characterized the compound's electronic properties, including its ability to donate and accept electrons. Additionally, a PubChem search identified an enantiomer with reported activity against threonyl-tRNA synthetase (ThrRS), a key enzyme involved in protein synthesis. Molecular docking studies further supported an interaction between the candidate compound and ThrRS, suggesting a potential mechanism of action that aligns with the observed cell cycle arrest. Moreover, pharmacokinetic profiling demonstrated the compound's high metabolic stability and moderate lipophilicity, further supporting its potential as a lead candidate for visceral leishmaniasis treatment.

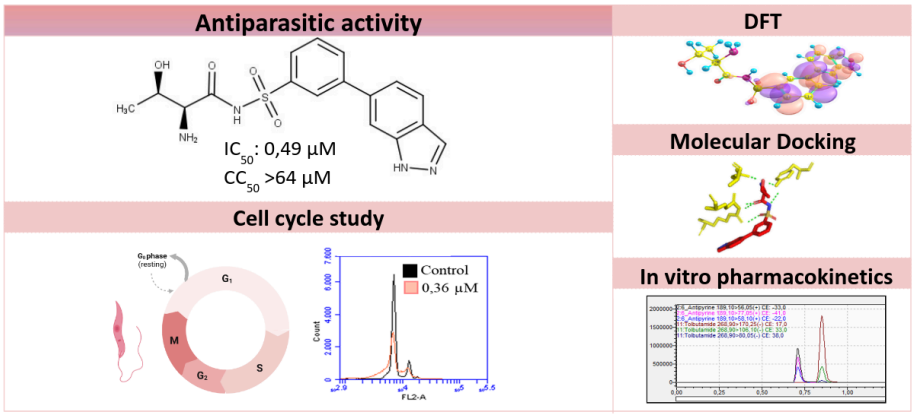

Figure 1 - Experimental schematic representation.

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