# Therapeutic Potential of Thiophene Derivative SB-200 against Leishmaniasis: Evaluation by Molecular Docking

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Leishmaniases are a group of significantly neglected tropical diseases, characterized by their severity and global prevalence. Currently, the available treatments for these diseases face substantial challenges, including high costs, considerable toxicity, the need for parenteral administration, and increasing parasitic resistance. Therefore, the search for therapeutic alternatives is crucial.In this context, the compound of interest is thiophene, a five-membered molecule with sulfur as a heteroatom and double bonds at positions 2 and 4, forming an aromatic system. Thiophene derivatives are relatively easy to synthesize and have been investigated due to their potential in combating Leishmania parasites, the causative agents of leishmaniases. One of these derivatives, SB-200, a 2-aminothiophene compound, has previously shown promising activity against *Leishmania (Leishmania) amazonensis*.The study aimed to assess the anti-Leishmania activity of SB-200 through an *in silico* approach using molecular docking techniques. Cellular targets were obtained from the Protein Data Bank, and the Autodock 4.2 package was employed for molecular docking procedures. The results revealed that SB-200 exhibits molecular affinity with crucial enzymes essential for the parasite's survival, including N-myristoyl transferase, leishmanolysin, and tryparedoxin peroxidase. These enzymes play vital roles in Leishmania, making them promising targets for the development of antiparasitic therapies.In the molecular docking process, 3D N-myristoyl transferase (4A30) structures were generated, defining a cubic box of 60x60x60 points with a spacing of 0.35 Å between grid points. Affinity grid centers were established. One hundred independent docking simulations were performed for each ligand, and the resulting conformations were grouped into families based on Root-Mean-Square Deviation (RMSD).Coordinates of the selected complexes were chosen based on the lowest energy docking conformation, combined with visual inspection. This study aims to deepen the understanding of interactions between N-myristoyl transferase and its ligands, contributing to research related to this protein and its potential therapeutic applications in combating leishmaniases. Therefore, the *in silico* approach and findings regarding SB-200 represent a crucial step in the development of new therapies for these neglected diseases.

**Key words**: Thiophenic derivative, Leishmaniasi, *Leishmania*, Molecular docking.

**Potencial Terapêutico do Derivado de Tiofeno SB-200 contra Leishmanioses: Avaliação por Docking Molecular**

As leishmanioses são graves doenças tropicais negligenciadas, com tratamentos caros, tóxicos e administrados via parenteral, além de resistência parasitária. O tiofeno, um composto de cinco membros com enxofre e duplas ligações, é estudado por sua eficácia contra Leishmania. O SB-200, derivado de tiofeno, exibiu promissora atividade anti-Leishmania, notadamente contra a *Leishmania amazonensis*. Este estudo in silico utilizou o docking molecular para avaliar a afinidade do SB-200 com enzimas cruciais para a sobrevivência do parasita, incluindo N-myristoyl transferase, leishmanolisina e triparedoxina peroxidase. Esses resultados destacam o potencial do SB-200 como candidato terapêutico contra as leishmanioses.

**Palavras-chave**: Thiophenic derivative, Leishmaniasi, Leishmania, Docking molecular
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