



INTEGRATED PLATFORM FOR RESEARCH AND ANALYSIS OF COMPOUNDS AGAINST LEISHMANIASIS: LEISHMOLDB

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ABSTRACT

Introduction: Open-access molecular databases have become crucial in advancing medicinal chemistry, providing researchers with access to vast collections of structural and biological data. These resources are especially important for exploring new treatments for neglected diseases like leishmaniasis. Yet, despite the urgent need for better options, existing treatments for this disease remain limited in effectiveness and safety. The high costs and low financial returns have also kept the pharmaceutical industry from investing in new solutions. This highlights a clear need for accessible, innovative tools that can strengthen research efforts and speed up the discovery of more effective therapies.

Objectives: LeishMolDB was developed as an integrated platform to support the research and analysis of new compounds with potential activity against *Leishmania* amastigotes, offering structural and biological information that optimizes research processes, saving both time and resources. By integrating computational chemistry tools with user-friendly interfaces, LeishMolDB aims to equip researchers with essential resources to evaluate the therapeutic potential of these compounds, paving the way for future treatments.

Methods: The selection process for molecules began with a detailed literature review focused on compounds with known IC₅₀ values against *Leishmania* amastigotes. The most active compounds were identified, carefully modeled in 3D, saved in .SDF format, and optimized for improved structural and functional analysis. The platform was designed for visual accessibility, utilizing HTML, JavaScript, and Tailwind CSS for front-end development, while Python and RDKit optimize data processing on the back end. In LeishMolDB, users can explore stored molecules, perform virtual screenings using Tanimoto coefficient calculations, and download 3D molecular structures for further research applications.

Results and Discussion: Currently, LeishMolDB contains 855 cataloged active molecules, accessible for virtual screening and detailed analysis, allowing researchers to explore potential treatments for leishmaniasis. The platform supports the addition of new molecules and offers five intuitive interfaces designed for easy navigation, data review, and structural comparisons, ensuring that the information is both accessible and valuable. The data review includes key metrics, such as Topological Polar Surface Area (TPSA) and Lipinski's Rule of Five, which help evaluate the drug-likeness of compounds. By incorporating Tanimoto coefficient similarity calculations, LeishMolDB enables users to identify molecular similarities, locate structural analogs, and highlight promising compounds for drug development. Collectively, these features position LeishMolDB as a valuable tool for the leishmaniasis research community.

Conclusion: LeishMolDB exemplifies a vital intersection between technology and medicinal chemistry, particularly valuable in leishmaniasis research. As a constantly updated platform, it provides researchers with an accessible resource that fosters collaboration, reduces research costs, and accelerates the development of essential treatments for leishmaniasis and other neglected diseases. LeishMolDB is poised to serve as a global resource that continuously supports advancements in drug discovery.