

## **An *in silico* functional annotation and screening of potential drug targets derived from *Leishmania* spp. hypothetical proteins identified by immunoproteomics**

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Leishmaniasis is a parasitic disease caused by the protozoan of the *Leishmania* genus. While no human vaccine is available, drugs such as pentavalent antimonials, pentamidine and amphotericin B are used for treat the patients. However, the high toxicity of these pharmaceuticals, the emergence of parasite resistance and/or their high cost have showed to the urgent need of identify new targets to be employed in the improvement of the treatment against leishmaniasis. In a recent immunoproteomics approach performed in the *Leishmania infantum* species, 104 antigenic proteins were recognized by antibodies in sera of visceral leishmaniasis (VL) dogs. Some of them were later showed to be effective diagnostic markers and/or vaccine candidates against the disease. Between these proteins, 24 considered as hypothetical were identified in the promastigote and amastigote-like extracts of the parasites. The present study aimed to use bioinformatics tools to select new drug targets between these hypothetical proteins. Their cellular localization was predicted to be seven membrane proteins, as well as eight cytoplasmic, three nuclear, one mitochondrial and five proteins remained unclassified. Their functions were predicted as being two transport proteins, as well as five with metabolic activity, three as cell signaling and fourteen proteins remained unclassified. Ten hypothetical proteins were well-annotated and compared to their homology regarding to human proteins. Two proteins, a calpain-like and clavaminase synthase-like proteins were selected by using Docking analysis as being possible drug targets. In this sense, the present study showed the employ of new strategies to select possible drug candidates, according their localization and biological function in *Leishmania* parasites, aiming to treat against VL.

**Keywords:** *Leishmania* spp.; bioinformatics tools; hypothetical proteins; drug targets; screening; immunoproteomics.

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