In silico exploration of the trypanothione reductase (TryR) of *L. mexicana*

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Human leishmaniasis is a tropical neglected disease which affects nearly 1.5 million people on a yearly basis. Perhaps one of the best known defense mechanisms of this type of parasite is supported by the polyamine metabolic pathway. As it provides the necessary compounds for its survival. Among the enzymes in this route, trypanothione reductase (TryR), an oxidoreductase enzyme, is crucial for the defensive mechanisms of the Leishmania genus against oxidative stress. Thus, it poses as an attractive target for drug development. The main drawback being the size of its catalytic pocket. Herein we present a computational study using structure-based methods to characterize the druggability of this target, beyond its catalytic site. Using a consensus methodology two pockets were found, with one of them being a putative cryptic site. We think these findings can help further drug design endeavors around trypanothione-related diseases.