

POSTER PRESENTATION

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# Repositioning of new potential schistosomicidal drugs using chemogenomic strategy

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## Background

Schistosomiasis remains a severe problem of public health in developing countries [1]. Several reports show that praziquantel, the drug of choice for treating schistosomiasis, can select *Schistosoma mansoni* strains resistant to the drug. Thus, developing new drugs against this parasitosis is a highly desirable goal [2]. In this context, enzymes involved in energetic metabolism could represent attractive drug targets for novel anti-schistosome chemotherapies [3,4]. We report a chemogenomic strategy for identification of approved drugs that may be able to interfere with energetic metabolism of the *Schistosoma mansoni*.

## Methods

The chemogenomic study was performed on a list containing 734 genes involved in oxidative phosphorylation (n = 45); nitrogen metabolism (n = 642); glycolysis (n = 11); citrate cycle (n = 10); and others (n = 26). Next, it was obtained from the GeneDB *S. mansoni* genome database individual information for genes (amino acid sequence in FASTA format, product name, and biological process). Each of these protein sequences was treated as a potential drug target and used to screen three freely available databases (DrugBank, STITCH 3.1, and TTD) based in the concept of the target sequence similarity. The targets with E-value score  $\leq 10^{-5}$  and score  $\geq 0.7$  were considered for further analyses.

## Results and conclusions

We were able to identify several drugs that are expected to interact with 6 targets involved in nitrogen metabolism (carbonic anhydrase II and carbonic anhydrase), citrate cycle

(succinate dehydrogenase), oxidative phosphorylation (ATP synthase delta chain and NADH-ubiquinone oxidoreductase mitochondrial precursor), and glutamate metabolism (glutaminase). One of these targets was associated with thiabendazole, whose activity has been previously evaluated against *S. mansoni*. [5]. However, 18 drugs were predicted to have activity against other targets and have never been evaluated against schistosome parasites (e.g., acetazolamide, doxorubicin, morantel tartrate, axantel pamoate, thiabendazole, and menthol). Our next step is to experimentally screen these drugs against *S. mansoni*. Being a cost and time saving route, drug repositioning is expected to accelerate the discovery of new anti-schistosome chemotherapies.

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