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Pharmacoinformatic approach for discovery of better drug combination with currently available drug against Leishmaniasis

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Hypoxanthine phosphoribosyl transferase (HGPRT; EC 2.4.2.8) is a central enzyme in the purine recycling pathway of all protozoan parasites. Protozoan parasites cannot synthesize purine bases (DNA/RNA) which is essential for survival as lack of de novo pathway. Thus, its good target for drug design and discovery as inhibition leads to cessation of replication. PRTase (transferase enzyme) has common PRTase type-I folding pattern domain for its activities. Genomic studies revealed the sequence pattern and identified highly conserved residues catalyzed the reaction in protozoan parasites. A recombinant protein has 24 kDa molecular mass (rLdHGPRT) was cloned, expressed and purified for testing of guanosine monophosphate (GMP) analogous compounds *in vitro* by spectroscopically to the rLdHGPRT, Lysates protein and MTT assay on *Leishmania donovani*. The predicted inhibitors of different libraries were screen into FlexX. The reported inhibitors were tested *in vitro*. The 2'deoxyguanosine 5' diphosphate (DGD) (IC_{50} value 12.5 µM) is two times more effective when compared to guanosine-5' diphosphate sodium(GD). Interestingly, LdHGPRT complex has showed stable after 24ns in molecular dynamics simulation with interacting amino acids are Glu125, Ile127, Lys87 and Val186. QSAR studies revealed the correlation between predicted and experimental values has shown R_2=0.985. Concludes that inversely proportional to their docked score with activities. It is predicted that patients suffering from both HIV and visceral leishmaniasis (VL) may benefit if they are treated with acyclovir in conjunction with first-line anti-leishmanial therapies such as Miltefosine and AmBisome.

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