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The screening of novel inhibitors against *Leishmania donovani* calcium ion channel to fight Leishmaniasis

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Leishmania is an intracellular protozoan parasite which causes Leishmaniasis, a global health problem affecting millions of people throughout 89 different countries in the world. The current treatment which includes use of Amphotericin B, antimonials and others has major drawbacks due to toxicity, resistance and extraordinary high cost. So there is an urgent need of development of new drug targets to fight against leishmaniasis. In this regard we have selected *Leishmania donovani* Ca^{2+} ion channel (Ld-CC) as potential drug target. Ld-CC regulates concentration of Ca^{2+} ions which is involved in several functions like flagellar motion, mitochondrial oxidative metabolism and entry inside the macrophages. Since Ld-CC has not been characterized yet, we performed homology modeling of *Leishmania donovani* Ca^{2+} ion channel (Ld-CC) and docking studies of ligand library against this channel. 542 compound library of National Cancer Institute (NCI) diversity 3 dataset selected for screening studies. The ligands ZINC17287336 and ZINC29590262 were selected as best energy conformers because they show highest binding affinity towards its target (Ld-CC). They interact with the active site residues in the pocket of Ld-CC which suggests that the docked conformations are good and acceptable. Moreover these two selected compounds also have relatively high binding affinity than nifedipine and verapamil, known human calcium channel blockers which had been reported to have mild anti-leishmanial activity. Among these two top screened inhibitors the ligand ZINC29590262 shows poor binding affinity towards the Human voltage-dependent L-type calcium channel subunit alpha-1C in comparison to the Ld-CC. Therefore we proposed this ligand as the best inhibitor which shows 40% more binding affinity with Ld-CC than the human-VDCC. These results suggest that our screened ligand ZINC29590262 could act as novel drug and may show much better anti-leishmanial activity.

Recent Publications

1. Arish M, Alaidarous M, et al. (2017) Implication of sphingosine-1-phosphate signaling in diseases: molecular mechanism and therapeutic strategies. *J Recept Signal Transduct Res*; 37(5): 437-446.
2. Kashif M, Manna P P, Akther Y, Alaidarous M, Rub A (2016) The Screening of novel inhibitors against *Leishmania donovani* Calcium ion channel to fight Leishmaniasis. *Infect Disord Drug Targets*; 17(2): 120-129.

Biography

Mohammed Alaidarous has received his PhD in Biochemistry from the University of Queensland, Australia in 2014. Presently he is an Assistant Professor in the Department of Medical Laboratory Sciences at Majmaah University in Saudi Arabia. His research interest is in understanding the molecular mechanism behind microbial pathogenesis by performing protein structural studies and has interest in structure-based drug and vaccine design.

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