Leonor Cervantes-Ceballos et al., Med Chem (Los Angeles) 2017, 7:8(Suppl)
DOI: 10.4172/2161-0444-C1-034

An In silico approach to discovering inhibitiors of trypanothione reductase from *leishmania* (viannia) *panamensis*.

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Leishmaniasis is the most prevalent neglected tropical diseases in many countries around the world. The identification and validation of molecular of targets can be a way to identify potential new drugs targets [1]. Trypanothione reductase (Try R) converts Trypanothione disulfide to the reduce Trypanothione dithiol and is the homolog of mammalian glutathione reductase, essentially involved in neutralization of host oxidative response [2]. The homology modeling of trypanothione reductase was performed using as a template the crystal structure from L. *infantum* (PDB ID: 2JK6). The homologous 3D structure was built using SWISS-MODEL. The stereochemical quality of 3D models was assessed by using PROCHECK. A molecular docking was performed from ZINC database; a total of 5000 was included. The virtual screening performed using Autodock; a total of 10 molecules presented a free binding energy to the Trypanothione reductase as potential drugs to fight this disease considered neglected. Among these compounds we can highlight three. Where, the compound number 792 (N-[(2R,3S,4R,5S,6S)-2-[1-[(2S,4aR,8aS)-6-[(3R,4aS,5S,6aR,7S,9aR,9bR)-5-hydroxy-3-(1-hydroxy-1-methyl),(free-binding energy 16,13 Kcal/mol) showed the best score. Our results may be helpful for further experimental investigations. Our study contributes the development of potent inhibitors for the treatment of leishmaniasis. This Research was supported by a grants from the University of Cartagena and Colciencias-Colombia, Project No. 512-2012; the National Program for Doctoral Formation Colciencias, 727- 2015 and Doctoral program in biomedical sciences from University of Cartagena.

Biography

Leonor Cervantes-Ceballos is PhD student in biomedical sciences from University of Cartagena (Colombia). Master in microbiology, associated to Chemical Research Group of Medicines of the University of Cartagena-Colombia.

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