Jairo Mercado-Camargo et al., Med Chem (Los Angeles) 2017, 7:8(Suppl)
DOI: 10.4172/2161-0444-C1-034

Homology modelling of different leishmanolysin (gp63) from *leishmania* spp. and molecular docking of flavonoids

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*Leishmania*sis is one of the world's neglected tropical diseases and it can consider as an important public health problem, endemic in 88 countries, caused by various species of *Leishmania* protozoans and more than 90 species of sand-flies as vectors (*Phlebotomus* spp. and *Lutzomyia* spp.). The molecular factors contribute to *Leishmania* spp. virulence and pathogenesis is the *major* surface protease, leishmanolysin (gp63), abundant in *Leishmania* promastigote and amastigote. Leishmanolysin protein was crystallized from L. *major* (code PDB: 1LML) using as a template to modelling different gp63 protein from *L. panamensis, L. braziliensis, L. donovani, L. mexicana and L. infantum.* The homologous 3D structure was built on the base of the crystal structure of 1LML using SWISS-MODEL and I-TASSER. The stereochemical quality of 3D models was assessed by using PROCHECK, ProSA-web, verify 3D and Molprobity. A molecular docking was performed with flavonoids retrieved from the natural product II database, a total of 5470 between flavonoids, chalcones and biflavonoids was included. The virtual screening performed using Autodock Vina from the PyRX 0.8 platforms; a total of 12 molecules presented a free binding energy to the leishmanolysin of L. major as potential drugs to fight this disease considered neglected. Among these compounds we can highlight the flavonoids rhuschalcone VI, epigallocatechin, agathisflavone, abyssinone IV, and quercetin (free-binding energy -8.6, -8.6, -8.4, -8.2 and, -8.2 kcal/mol, respectively) among others. Our results may be helpful for further experimental investigations.

Biography

Jairo Mercado-Camargo PhD student in biomedical sciences from University of Cartagena (Colombia). Assistant professor in analytical chemistry and spectroscopy of the Program of Pharmaceutic Chemistry at the University of Cartagena (Colombia). This training initiated over 5 years with experience in develops medicinal chemistry & computer aided drug designing.

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