In silico screening of volatile compounds which can complex with the AeagOBP1 odor-binding protein of Aedes aegypti L.

Tarcisio Silva Melo[1], Liliane Pereira de Araújo[1], Rosangela Santos Pereira[1], Thaís Almeida de Menezes[2], Wagner Rodrigues de Assis Soares[1], Bruno Silva Andrade[1]

1 UNIVERSIDADE ESTADUAL DO SUDOESTE DA BAHIA
2 UNIVERSIDADE ESTADUAL DE FEIRA DE SANTANA

Abstract

Several species of medicinal plants generally contain in their composition volatile compounds. In general, these organic molecules act as repellents or attractive of pollinating insects. The aim of this work was to prospect new attractive compounds for Aedes aegypti L. through the Odorant Binding Protein (AeagOBP1). The AeagOBP1 structure was downloaded from PDB Database, with access code 3K1E considering the organism, resolution (1.85) and R-value (0.212). Structures of isolated compounds from semi arid plants were drawn using Marvin Sketch (Chemaxon). After, we verified valences, structural erros, and then we saved all ligands in MOL2 format. For docking studies, all ligands were prepared using AutoDock tools and saved in PDBQT format. Furthermore, we defined the active stite region (gridbox) for AeagOBP1 and saved the coordinates. Molecular docking calculations were performed using AutoDock Vina. After evaluated each docking positions, and cosidering best affinity energy and ligand positing inside AeagOBP1 active pocket, we used PyMOL 1.7 in order to save complexes in PDB format. 2D interaction maps for each complex were generated using Discovery Studio 4.0. In this work we tested 9 molecules deposited in the Semi Arid Molecules Database (SAM Database), hosted on the servers of the Bioinformatics and Computational Chemistry Lab (LBQC-UESB). SAM3814 ligand had best interaction with AeagOBP1 (-8.3 Kcal/mol). Standard ligands were tested for validation purposes: Carbon dioxide (-1.6 Kcal/mol), lactic acid (-3.2 Kcal/mol), octenol (-4.6 Kcal/mol) and 2-oxopentanoic acid (-4.2 Kcal/mol), however presented worst interaction energies when compared to SAM3814. This work demonstrated that natural volatile compounds isolated from Brazilian semi arid plants could act as new ligand prototypes in order to develop new attractive and/or repellent compounds for Aedes aegypti mosquito. On the other hand, this could be used as an new strategy for the controlling incidence of dengue, chikungunya and zika viruses.

Funding: Sem financiamento