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In silico inhibitors for falcipain-3 in *Plasmodium falciparum*

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ABSTRACT

*Saddala MS, Gayathri P, Obaiah J, Vallamma C, Usha Rani A., In silico inhibitors for falcipain-3 in Plasmodium falciparum, Onl J Bioinform., 14 (3): 293-301, 2013.*Inhibition of falcipain-3 prevents maturation of *Plasmodium falciparum*, suggesting that the protein could be a target for antimalarial activity. Falcipain-3was energy minimized and subjected to molecular dynamics simulations using NAMD 2.9 software with CHARMM27 force field in water and the receptor structure was minimized with 25,000 steps for 500ps and simulated 10,000 steps for 2ns. 2500 compounds were screened from PubChem database through structure based Virtual screening by referencing Mefloquine. The screened compounds were docked into the active site of the protein using Autodock Vina in PyRx Virtual Screening tool. Results showed that CID3000506, CID40468067, CID65330, CID40692 and CID4046had a highest binding energyof-9.4, -8.9, -8.4, -7.9 and -7.2 kcal/mol, respectively. Lead hit compounds were tested for toxicity and bioavailability with Osiris and Molinspiration online servers. Active site amino acidsHis18, Asp44, Tyr63, Gln110, Tyr115, Asp168, His196, Glu199, Gly453 and Met434could play a role in binding and catalytic activity.

KEYWORDS: Falcipain-3, simulations, docking, PubChem database, Autodock Vina

INTRODUCTION

Malaria is one of the most important infectious diseases in the world wide and affects about 40% of the world's population (Breman, 2001).It is caused by different species of *Plasmodium*. Four *Plasmodium* species have been well known to cause human malaria, namely,