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Research and Development in Pharmacy & Life Sciences Abstract

In Silico and Whole Cell-based In vitro screening of Flavonoids from Citrus species towards the identification of Antimalarial Lead(s) and Prediction of Mode of Action

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Abstract:

Development of resistance by the malaria parasite *Plasmodium falciparum* has put challenges in the eradication of deadly malaria disease. Hence, newer strategies are being considered to combat this disease and research programmes with the target of new lead identification are going on worldwide to develop new chemotherapeutic agents. In this study, flavonoids found mainly in the fruits of *Citrus* species having traditional use in malaria-associated fever were selected for *in silico* multiple-target directed screening against three vital targets of the parasite namely, dihydrooroate dehydrogenase (*Pf*DHODH), dihydrofolate reductase thymidine synthase (*Pf*DHFR-TS) and plasma membrane P-type cation translocating ATPase (*Pf*ATP4) to find out new lead molecule(s). The *in silico* screening was carried out using different protocols of the Biovia Discovery Studio 2018 software and Network analyzer plugin of Cytoscape 3.6.0 followed by *in vitro* screening of the best lead. The selected lead was found to have good binding affinity against *Pf*DHODH and *Pf*ATP4 with –CDocker energy 42.2719 and 33.1447 with respect to their co-crystal ligands. These findings were also supported by Structure-based Pharmacophore, DFT (Density Functional Theory) study and also by *in vitro* evaluation of the lead which showed IC_{50} value of 8.23 µm and 12.41 µm against 3D7 (chloroquine-sensitive) and RKL-9 (chloroquine-resistant) strain of *P. falciparum* respectively. This study could identify a moderately active lead molecule with prediction of mode of action. The research outcome can be utilized to design new antimamarial compounds by targeting the two enzymes.

Biography:

Neelutpal Gogoi obtained his Master of Pharmacy degree in 2015 from Dibrugarh University and currently engaged in research as Ph.D. Scholar in the Department of Pharmaceutical Sciences, Dibrugarh University. He has received Fellowship under 'Young Scientist' category from the Department of Health Research, Ministry of Health & Family Welfare, Govt. of India to carry out his doctoral study.

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