In Silico docking analysis to identify potent inhibitors from the extract of *Eucalyptus tereticornis* against malarial proteins

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ABSTRACT

Malaria is a lethal disease caused by protozoan parasite of Genus *Plasmodium* which affects 9.27 million people and takes a toll of 40,297 every year in India. As these parasites are having the capability of developing resistance to currently used drugs, it is essential to identify new antimalarial natural drug having no side effects. *Eucalyptus tereticornis* is famous for its antiseptic property but, the recent literature studies revealed that it also posses anti malarial properties. In the current investigation, a study was conducted to search and predict effective anti-malarial lead compounds from *E. tereticornis*. From the study, disease causing proteins present in the parasites were recognized as potential target and five new plant compounds possessing antimalarial activity were identified as inhibitors. *In Silico* molecular docking were performed between target proteins and there inhibitors. The 3D structures of the targets and inhibitors were retrieved from PDB and Pubchem for further analysis. The Ten target proteins – Five ligands' interaction studies were performed and its ADME properties were also checked. The docking result revealed a particular target showing best binding affinity with all the inhibitors when compared with other targets. Further, this study can be implemented to *in vitro* and *in vivo* analysis thereby helping in development of novel drug against malaria.

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