In Silico Studies on Selected Drug Targets for Combating Drug Resistance in Plasmodium Falcifarum

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Abstract : With drug resistance becoming widespread in Plasmodium falciparum infections, development of the alternative drugs is the desired strategy for prevention and cure of malaria. Three drug targets were selected to screen promising drug molecules from the GSK library of around 14000 molecules. Using an in silico structure-based drug designing approach, the differences in binding energies of the substrate and inhibitor were exploited between target sites of parasite and human to design a drug molecule against Plasmodium. The docking studies have shown several promising molecules from GSK library with more effective binding as compared to the already known inhibitors for the drug targets. Though stronger interaction has been shown by several molecules as compare to reference, few molecules have shown the potential as drug candidates though in vitro studies are required to validate the results.