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In silico epitope prediction, vaccine studies and identification of inhibitors against secretory proteins of *Plasmodium falciparum*

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Malaria is one of annihilating problem caused by Plasmodium infection. Due to non-availability of any effective vaccine and development of drug resistance against the existing drugs malaria could not be eradicated completely. Therefore there is an urgent need to search for new alternative drug targets or vaccine candidates. To outcompete this we pored over secretory proteins of plasmodium which are secreted out from the infected erythrocyte, and which is one of the strategies that parasite utilize to evade the host immune system. Therefore we hypothesize the involvement of secretory proteins in host immune modulation or in parasite invasion process. Secretory proteins therefore might serve both as good drug target or vaccine candidates. Our present study is aimed to predict the 3D structure of secretory proteins of Plasmodium falciparum and we have also performed In-silico screening of diverse drug like molecules against these proteins. The virtual screening leads to the retrieval of some of the top compounds which were evaluated for their in-vitro anti-malarial activity against Plasmodium falciparum 3D7 strain. We have identified four compounds with less than 100 nM IC₅₀. We have also predicted epitopes present in the proteins through different tools like PROPRED, and PREDEP for T cell epitope and BCPRED for Linear B cell epitope. Out of all predicted epitopes one antigenic peptide was selected on the basis of antigenicity, surface accessibility, hydrophilicity, and it is synthesized for in-vitro vaccine studies. Synthetic peptide was used for the immunization of mice and for the detection of cytokine profiling in immunized mice.

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