### Centre for High Performance Computing 2021 National Conference

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# Screening FDA-approved drugs and natural compounds to hemozoin biomineralization inhibitors in P. falciparum

Malaria has been targeted by the WHO for elimination for well over a decade now. The emergence of resistance to widely used antimalarials combined with the persistence and lack of drugs that target other Plasmodium species like P. vivax has made it challenging to eradicate malaria.

The main aim of this research is to find drugs that inhibit the function of a lipocalin that has been shown to be involved in hemozoin biomineralization.1 The study will focus on the virtual screening of existing compounds from public databases as potential inhibitors of P. falciparum lipocalin (PfLCN). The screening and understanding of binding and protein ligand dynamics will require docking, free energy calculations and molecular dynamics simulations.

#### Student?

Yes

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