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Development of target focused library against drug target of *P. falciparum* using SVM and Molecular docking

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PfHslV, a homolog of β subunit of 20S proteasome forms the proteolytic core of the *PfHslUV* machinery in *P. falciparum* [1,2]. *PfHslV* has no homolog in the human host and it is a promising drug target essential to the plasmodial metabolism. The use of single proteasome inhibitor targeting these threonine proteases has a potential to be antimalarial drug candidate. One of our recent studies identified several promising inhibitors against 20S β5 subunit of *P. falciparum* [3]. The present study adopts a similar knowledge based virtual screening strategy using Support Vector Machines (SVM) and molecular docking to build a focused library of potential *PfHslV* inhibitors. SVM model has been trained using 170 molecular descriptors of 64 inhibitors and 208 putative non-inhibitors. The non-linear classifier based on Radial Basis Function (RBF) kernel yielded classification accuracy of 97%. The SVM model rapidly predicted inhibitors from NCI library and were subsequently docked in to the active site of an optimised three-dimensional model of *PfHslV*. The novel drug-like *PfHslV* inhibitors with very good binding affinity and novel scaffold can be a good starting point to develop new antimalarial drugs.

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