Molecular Modelling of Calcium Dependent Protein Kinase 4 (CDPK4) from *Plasmodium falciparum*

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ABSTRACT

Malaria continues to be one of the most serious global health challenges. The increasing incidence of drug resistant *Plasmodium* strains has emphasised the need for urgent action in the development of new therapeutic strategies against this disease. Development of new drug targets is of vital importance in this regard. The recent availability of genomic information and the resultant observation that in many instances, protein kinases from parasitic protozoa are phylogenetically distant from those in humans has established this group of enzymes as potential drug targets in the Malaria parasite. One of the differences from the host kinome identified in *Plasmodia* was the presence of calcium dependent protein kinases (CDPKs), normally only found in plants. In order to rationally design novel inhibitors and chemical tools exclusively targeting CDPKs, reliable molecular structures are needed. High resolution structures will also enable *in silico* screening to identify new leads. Structural Bioinformatics, specifically molecular modelling, can contribute immensely to improving access to structural information for these challenging targets. Here, a three dimensional structure of *Pf*CDPK4 created by homology modelling is reported. Further, the model is used as a receptor for *in silico* screening of a large chemical library. Future work will aim to screen a prioritised subset of the library *in vitro* and to study the structures of *Pf*CDPK4 in complex with identified hits by X-ray crystallography.