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Plasmodium falciparum Phosphatidylinoistol-4-kinase enzyme: Homology modelling and structure-based characterisation of the binding pocket.

The Plasmodium falciparum phosphatidylinositol 4-kinase type III beta (PfPI4KIIIβ), a protease kinase enzyme, has been shown to be vitally important for the survival of the malaria parasite, both in the host and the vector. However, the lack of the three-dimensional structure and the full structural characterisation of its binding pocket limits its utility and subsequently the development of new, selective and highly efficacious inhibitors. Thus, the current study is employing a homology modelling and docking strategy in analysing the binding site morphology and key amino acids that are involved in ligand-substrate complex formation. Our results reveal a stable homology model whose stability, before and after molecular dynamics, is confirmed by Ramachandran plot and RMSD graph . Furthermore, docking a number of reported PfPI4K inhibitors on this model revealed that the binding pocket of PfPI4KIIIβ is hydrophobic and prefers hydrophobic ligands who adopt twisted conformations. Secondly, a number of docked ligands also showed interesting interactions with key amino acids as a results of functional groups making up the In conclusion we have developed a homology model that allows for the characterisation of the binding sites as well as the analysis of the key amino acid residues involved in ligand-substrate complex formation.

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