Molecular modeling of the *Plasmodium falciparum* pre-mRNA splicing and nuclear export factor PfU52

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ABSTRACT

UAP56/SUB2 is a DExD/H-box RNA helicase that is critically involved in pre-mRNA splicing and mRNA nuclear export. This helicase is broadly conserved and essential in many eukaryotic lineages, including protozoan and metazoan parasites. Previous research suggests that helicases from parasites could be promising drug targets for treating parasitic diseases. Accordingly, characterizing the structure and function of these proteins is of interest for structure-based, *de novo* design of new lead compounds. Here, we used homology modeling to construct a three-dimensional structure of PfU52 (PMDB ID: PM0079288), the *Plasmodium falciparum* ortholog of UAP56/SUB2. Comparative *in silico* analysis revealed that although PfU52 shared many physicochemical, structural and dynamic similarities with its human homolog, it also displayed some unique features that could be exploited for drug design.