## Egress and Invasion Machinery of Malaria: An In-depth Look into The

## Structural and Functional Features of The Flap Dynamics of Plasmepsin

## IX and X

## **Supplementary Material**

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PLASMEPSIN	TEMPLATE	SEQUENCE IDENTITY	Z-SCORE
IX	4OBZ	35%	-6.16
Χ	4OBZ	35%	-6.22
Table S1 The Z-score	and sequence identity o	$f_{4}OBZ$ template used f	or Plm IX-X



Figure S1. Ramachandran plots for models Plm IX (left) and Plm X (right).



**Figure S2.** Overall model quality generated using ProSA-web of Plm IX (left) and Plm X (right).



**Figure S3.** Superimposed image of Plasmepsins I (PDB: 3QRV; red), II (PDB:1LF4, orange red), III (PDB: 3FNS, orange), IV (1LS5, green), VI (dark green), VII (cyan), IX (sea green) and X (blue).

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Figure S4. Sequence alignment of Plasmepsin I-X from *Plasmodium falciparum*.



Figure S5. RMSD plot of plasmepsin IX and X, displaying system stability after 30ns.



PE= -163213,16136

PE= -158461,37335

**Figure S6**. Potential energy (PE) plots of Plm IX (left) and Plm X (right) with interaction cutoff of 12 Å. Mean values are presented below the respective plots.