
Supplementary information

The molecular basis for sugar import in malaria parasites

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Supplementary Information

1. MD simulation table details

Initial model	Initial lipid configuration	POPC molecules	Solvent molecules (water, Na, Cl)	Total number of atoms	Ligand	Duration (ns)	Ligand displacement from binding site
<i>Pf</i> HT1	1	245	21,587 - 101 - 104	105,448	-	1000	-
<i>Pf</i> HT1	2	245	21,653 - 101 - 104	105,646	-	550	-
<i>Pf</i> HT1	3	245	21,562 - 101 - 104	105,373	-	650	-
<i>Pf</i> HT1	1	245	21,584 - 101 - 104	105,463	D-glucose	1000	no
<i>Pf</i> HT1	2	245	21,650 - 101 - 104	105,661	D-glucose	1000	no
<i>Pf</i> HT1	3	245	21,559 - 101 - 104	105,388	D-glucose	1000	partial
hGLUT3	1	247	20,258 - 96 - 98	101,385	-	1000	-
hGLUT3	2	247	20,239 - 96 - 98	101,328	-	424	-
hGLUT3	3	247	20,239 - 96 - 98	101,442	-	350	-
hGLUT3	1	247	20,257 - 96 - 98	101,406	D-glucose	1000	yes
hGLUT3	2	247	20,238 - 96 - 98	101,349	D-glucose	1000	yes
hGLUT3	3	247	20,276 - 96 - 98	101,463	D-glucose	1000	yes

2. Uncropped gel of extended data fig. 2a.

