



PharmMapper predictions and their respective homologues in *Plasmodium falciparum*

PDB ID	Target Name	FI Score	Normalized FI Score	Organism	Homologue in <i>P. falciparum</i>	Coverage	E value	Identity	Accession
1U40	L-lactate dehydrogenase	3.541	0.3219	<i>Plasmodium falciparum</i>	L-lactate dehydrogenase	—	—	—	XP_001340989.1
1V00	Protein kinase S	2.52	0.252	<i>Plasmodium falciparum</i>	protein kinase S	—	—	—	XP_001350280.1
1RDW	Actin, alpha skeletal muscle	2.514	0.2514	<i>Oryzotoglossus canaliculus</i>	actin I	99%	0	82%	XP_001350847.1
1OM1	Casain kinase II subunit alpha	5.057	0.3371	<i>Zea mays</i>	casain kinase II, alpha subunit	96%	1.00E-154	69%	XP_001347771.1
3BM9	Heat shock protein HSP 90, alpha	3.13	0.4141	<i>Homo sapiens</i>	heat shock protein 86	97%	0	64%	XP_001348998.1
1BOA	Methionine aminopeptidase 2	3.517	0.4397	<i>Homo sapiens</i>	methionine aminopeptidase	80%	7.00E-153	58%	XP_001348501.1
3F7Z	Glycogen synthase kinase-3 beta	4.223	0.4223	<i>Homo sapiens</i>	glycogen synthase kinase-3 beta	76%	4.00E-136	55%	XP_001351197.1
2CSN	Casain kinase I homolog 1	2.354	0.4256	<i>Schizosaccharomyces pombe</i>	casain kinase I	63%	6.00E-111	54%	XP_020433862.1
1VC2	Glycerinaldehyde-3-phosphate dehydrogenase	3.639	0.2599	<i>Thromus thermophilus</i>	aldehyde-3-phosphate dehydrog	96%	4.00E-107	52%	XP_001348772.1
2UZ1	Glycerinaldehyde-3-phosphate dehydrogenase	3.716	0.3716	<i>Bis staurus</i>	pendent protein kinase catalyti	90%	2.00E-114	50%	XP_001352213.1

Homology modeling details

<i>P. falciparum</i> target	PDB (ID)/homology model	Resolution	Template ID	Template name	Coverage	Identity
L-lactate dehydrogenase	PDB (5XU)	1.7	—	—	—	—
protein kinase S	PDB (1V00)	1.9	—	—	—	—
actin I	PDB (GCRU)	1.3	—	—	—	—
casain kinase II, alpha subunit	PDB (5XVU)	3.0	—	—	—	—
heat shock protein 86	Homology model	5.6d	—	Heat shock protein 90 beta	92%	69%
methionine aminopeptidase	Homology model	5c8	—	Methionine aminopeptidase 2	58%	59%
Glycogen synthase kinase-3 beta	Homology model	4e7w	—	Glycogen Synthase Kinase 3	81%	49%
casain kinase I	Homology model	5fgd	—	Casain kinase I alpha	100%	63%
glyceraldehyde-3-phosphate dehydrogenase	PDB (2BAR)	2.25	—	—	—	—
MP-dependent protein kinase catalytic subu	Homology model	39m	—	cAMP-dependent protein kinase catalytic subunit alpha	96%	51%

Statistical validation of homology models

<i>P. falciparum</i> target	Favored rotamers	Ramachandran outliers	Ramachandran favored	Clashscore	MaxProbity score
L-lactate dehydrogenase	—	—	—	—	—
actin I	—	—	—	—	—
casain kinase II, alpha subunit	—	—	—	—	—
heat shock protein 86	98.3%	0.1%	97.6%	7.32	1.48
methionine aminopeptidase	98.5%	0.3%	96.7%	5.98	1.53
Glycogen synthase kinase-3 beta	97.7%	0.0%	98.5%	6.18	1.43
casain kinase I	97.3%	0.0%	97.6%	7.46	1.54
glyceraldehyde-3-phosphate dehydrogenase	—	—	—	—	—
MP-dependent protein kinase catalytic subu	98.6%	0.0%	97.1%	7.28	1.26

Docking scores

<i>P. falciparum</i> target	Grid Dimensions (x,y,z)	28a	28b	28c	28d	28f	28g	28i	28k	28l
L-lactate dehydrogenase	35.3 x 11.74 x 17.30	-5.07	-3.79	-5.10	-4.36	-5.67	-4.55	-3.91	-3.49	-5.26
protein kinase S	21.00 x 4.24 x 33.95	-8.76	-8.00	-8.87	-8.36	-8.33	-9.31	-6.25	-8.24	-9.10
actin I	21.00 x 4.24 x 33.95	-8.76	-8.00	-8.87	-8.36	-8.33	-9.31	-6.25	-8.24	-9.10
casain kinase II, alpha subunit	3.85 x 6.72 x 13.62	-6.33	-5.75	-7.06	-6.01	-5.59	-5.83	-4.71	-4.07	-7.84
heat shock protein 86	175.54 x 176.34 x 137.02	-5.38	-5.93	-5.48	-5.96	-5.20	-5.79	-5.48	-4.04	-5.84
methionine aminopeptidase	27.38 x 20.08 x 17.83	-7.89	-8.00	-7.38	-8.77	-7.15	-7.13	-7.41	-8.39	-7.60
Glycogen synthase kinase-3 beta	93.81 x 68.05 x 9.74	-7.95	-7.92	-7.91	-7.89	-8.00	-6.27	-6.56	-8.06	-8.07
casain kinase I	3.84 x 7.08 x 14.00	-5.50	-5.10	-5.61	-4.78	-5.12	-5.86	-4.23	-4.77	-6.78
glyceraldehyde-3-phosphate dehydrogenase	16.93 x 21.00 x 14.07	-5.54	-6.15	-5.95	-5.92	-5.12	-6.26	-6.14	-5.87	-6.92
MP-dependent protein kinase catalytic subu	26.00 x 8.67 x 21.11	-5.91	-5.71	-6.68	-6.20	-5.95	-6.60	-5.38	-5.55	-7.13