

## Supplementary data for Toomey *et al.* “Genomes2Drugs: identifies target proteins and lead drugs from proteome data”.

### Supplementary Table S1: Genomes2Drugs search of the *Plasmodium falciparum* proteome.

The FASTA formatted proteome of the malarial parasite *P. falciparum* strain 3D7 was downloaded from EMBL-EBI Interg8. The Genomes2Drugs output was sorted by  $R_{\text{huPDB}}$ . Numerous fields have been removed and abridged for clarity. Putative, uncharacterised proteins likely to be good targets for further analysis are highlighted in blue. PDB homologue titles containing the word ‘plasmodium’ are highlighted in yellow. DrugBank hits associated with malaria, according to NCBI PubMed, are highlighted in green.

query_title	$R_{\text{huPDB}}$	$R_{\text{huPDB}}$ Rank	human_accession	human_ expect	pdb_title	pdb_ expect	drugbank_title	drugbank_ expect
tr Q7KQK5 Q7KQK5_PLAF7 Apical membrane antigen 1	180.6	1	HEXB_HUMAN	3.8	pdb1Z40IE Chain E, Ama1 From <b>Plasmodium Falciparum</b>	1E-180	2783_all_target_protein.fasta Apical merozoite antigen 1 (DB03366)	1E-180
tr Q8IBE8 Q8IBE8_PLAF7 Erythrocyte binding antigen	178.4	2	Q8N9N0	0.026	pdb1ZROIB Chain B, Crystal Structure Of Eba-175 Region Ii (Rii) Crystallized In The Presence Of (Alpha)2,3-Sialyllactose	1E-180	1688_all_target_protein.fasta <b>NADH dehydrogenase</b> [ubiquinone] 1 subunit C2 (DB00157; DB01136)	0.48
tr Q6LFB9 Q6LFB9_PLAF7 Enoyl-acyl carrier reductase	170.7	3	PECR_HUMAN	0.046	pdb1VRWIB Chain B, Crystal Structure Analysis Of <b>Plasmodium Falciparum</b> Enoyl-Acyl-Carrier-Protein Reductase With Nadh	1E-172	44_all_target_protein.fasta <b>Enoyl-acyl carrier reductase</b> (DB01907)	1E-180
tr Q8ILB1 Q8ILB1_PLAF7 NAD(P)H-dependent glutamate synthase, <b>putative</b>	165.9	4	DPYD_HUMAN	7E-15	pdb1EA0IB Chain B, Alpha Subunit Of A. Brasilense Glutamate Synthase	1E-180	38_all_target_protein.fasta Ferredoxin-dependent glutamate synthase 2 (DB02926; DB03247; DB04184)	1E-180
tr Q8IJH3 Q8IJH3_PLAF7 Orotidine 5'-phosphate decarboxylase	162.5	5	PYR5_HUMAN	0.32	pdb2F84IA Chain A, Crystal Structure Of An Orotidine-5'-Monophosphate Decarboxylase Homolog From <b>P.Falciparum</b>	1E-163	2452_all_target_protein.fasta <b>Orotidine 5'-phosphate decarboxylase</b> (DB01915; DB02202; DB02309; DB02890; DB02957; DB03403; DB03685; DB03718)	0.0002
tr Q8I5F4 Q8I5F4_PLAF7 <b>Putative uncharacterized</b> protein	156.4	6	AHNK_HUMAN	2.7	pdb2B30ID Chain D, Initial Crystallographic Structural Analysis Of A Putative HadCOF-Like Hydrolase From <b>Plasmodium Vivax</b>	1E-156	4342_all_target_protein.fasta Phosphoglycolate phosphatase (DB01942)	2E-07
tr Q8ILT0 Q8ILT0_PLAF7 NADP-specific glutamate dehydrogenase	151.5	7	DHE4_HUMAN	3E-29	pdb2BMAIF Chain F, The Crystal Structure Of <b>Plasmodium Falciparum</b> Glutamate Dehydrogenase, A Putative Target For Novel Antimalarial Drugs	1E-180	67_all_target_protein.fasta <b>Glutamate dehydrogenase</b> (DB01907)	2E-36
tr Q8ILJ7 Q8ILJ7_PLAF7 Phosphoenolpyruvate carboxylase	148.8	8	VTDB_HUMAN	6.3	pdb1JQOIB Chain B, Crystal Structure Of C4-Form Phosphoenolpyruvate Carboxylase From Maize	1E-148	2554_all_target_protein.fasta Phosphoenolpyruvate carboxylase (DB04317)	1E-130
tr Q8I3X4 Q8I3X4_PLAF7 Uridine phosphorylase, <b>putative</b>	143.5	9	UPP2_HUMAN	3	pdb1Q1GIF Chain F, Crystal Structure Of <b>Plasmodium Falciparum</b> Pnp With 5'-Methylthio-Immucillin-H	1E-143	3815_all_target_protein.fasta Uridine phosphorylase, putative (DB03743; DB03881; DB04402)	1E-144
tr Q76NM3 Q76NM3_PLAF7 L-lactate dehydrogenase	141.8	10	LDHC_HUMAN	6E-39	pdb1CEQA Chain A, Chloroquine Binds In The Cofactor Binding Site Of <b>Plasmodium Falciparum</b> Lactate Dehydrogenase	1E-180	2579_all_target_protein.fasta <b>L-lactate dehydrogenase</b> (DB01907; DB02111; DB02401; DB02737; DB03162; DB03940; DB04640; DB04641)	1E-180

tr Q8IB03 Q8IB03_PLAF7 Putative uncharacterized protein PF08_0063	138.6	11	CLPB_HUMAN	4E-42	pdb11QVRIC Chain C, Crystal Structure Analysis Of Clpb	1E-180	1453_all_target_protein.fasta Chaperone clpB (DB04395) 1877_all_target_protein.fasta Transketolase 1 (DB01658; DB01682; DB01987; DB02814; DB03937)	1E-180
tr Q6LFF9 Q6LFF9_PLAF7 Transketolase, putative	138.3	12	TKT_HUMAN	2E-42	pdb11GPUIB Chain B, Transketolase Complex With Reaction Intermediate	1E-180	2060_all_target_protein.fasta Plasmepsin-2 (DB02505; DB03063; DB04373; DB04378)	1E-161
tr Q8IM16 Q8IM16_PLAF7 Plasmepsin, putative	135.9	13	CATD_HUMAN	8E-45	pdb11LS5IB Chain B, Crystal Structure Of Plasmepsin Iv From <i>P. Falciparum</i> In Complex With Pepstatin A	1E-180	1716_all_target_protein.fasta Phosphoenolpyruvate carboxykinase [ATP] (DB02737; DB03431; DB04184)	1E-113
tr Q8IDR1 Q8IDR1_PLAF7 Phosphoenolpyruvate	135.4	14	PTN13_HUMAN	2.7	pdb11II2IB Chain B, Crystal Structure Of Phosphoenolpyruvate Carboxykinase (Pepck) From <i>Trypanosoma Cruzi</i>	1E-135	2060_all_target_protein.fasta Plasmepsin-2 (DB02505; DB03063; DB04373; DB04378)	1E-180
tr Q8I6V3 Q8I6V3_PLAF7 Plasmepsin 2	132.3	15	CATD_HUMAN	2E-48	pdb12BJUIA Chain A, Plasmepsin Ii Complexed With A Highly Active Achiral Inhibitor	1E-180	2060_all_target_protein.fasta Plasmepsin-2 (DB02505; DB03063; DB04373; DB04378)	1E-180
spl Q7KQM4 PLM1_PLAF7 Plasmepsin-1	129.5	16	RENI_HUMAN	3E-51	pdb12BJUIA Chain A, Plasmepsin Ii Complexed With A Highly Active Achiral Inhibitor pdb12BMAIF Chain F, The Crystal Structure Of <i>Plasmodium Falciparum</i> Glutamate Dehydrogenase, A Putative Target For Novel Antimalarial Drugs	1E-180	67_all_target_protein.fasta Glutamate dehydrogenase (DB01907) 2060_all_target_protein.fasta Plasmepsin-2 (DB02505; DB03063; DB04373; DB04378)	6E-51
tr Q8IM15 Q8IM15_PLAF7 HAP protein GN=PF14_0078	119.6	18	RENI_HUMAN	4E-36	pdb12BJUIA Chain A, Plasmepsin Ii Complexed With A Highly Active Achiral Inhibitor	1E-155	4308_all_target_protein.fasta Adenosine deaminase (DB02096; DB02616; DB02830; DB03015; DB03220; DB03370; DB03572)	1E-155
tr Q8IJA9 Q8IJA9_PLAF7 Adenosine deaminase, putative	116.3	19	ADA_HUMAN	2E-22	pdb12AMXIB Chain B, Crystal Structure Of <i>Plasmodium</i> Yoelii Adenosine Deaminase (Py02076)	1E-138	1453_all_target_protein.fasta Chaperone clpB (DB04395)	8E-26
tr Q8IIJ8 Q8IIJ8_PLAF7 Heat shock protein 101, putative	114.0	20	CLPB_HUMAN	1E-37	pdb11QVRIC Chain C, Crystal Structure Analysis Of Clpb pdb11KZHIB Chain B, Structure Of A Pyrophosphate-Dependent Phosphofructokinase From The Lyme Disease Spirochete <i>Borrelia</i> <i>Burgdorferi</i>	1E-151	1300_all_target_protein.fasta 6- phosphofructokinase (DB02726; DB04493)	1E-152
tr Q8I2Z8 Q8I2Z8_PLAF7 6-phosphofructokinase, putative	111.3	21	K6PL_HUMAN	0.002	pdb11TV5IA Chain A, <i>Plasmodium Falciparum</i> Dihydroorotate Dehydrogenase With A Bound Inhibitor	1E-114	3153_all_target_protein.fasta Dihydroorotate dehydrogenase homolog, mitochondrial (DB00263; DB00359; DB00664; DB01145)	8E-11
spl Q08210 PYRD_PLAF7 Dihydroorotate dehydrogenase homolog, mitochondrial tr Q8I2S7 Q8I2S7_PLAF7 3-oxoacyl-(Acyl-carrier protein) reductase, putative	110.3	22	PYRD_HUMAN	2E-70	pdb12C07IA Chain A, Oxoacyl-Acp Reductase Of <i>Plasmodium Falciparum</i>	1E-180	3052_all_target_protein.fasta 3- oxoacyl-[acyl-carrier-protein] reductase (DB03461)	1E-180
tr Q8IEU2 Q8IEU2_PLAF7 <i>Plasmodium falciparum</i> gamete antigen 27/25	106.6	23	DHB8_HUMAN	4E-43	2135_all_target_protein.fasta Voltage-dependent L-type calcium channel subunit alpha-1C (DB00270; DB00308; DB00622; DB00653; DB00661; DB01388)	1E-149		7E-66
	105.7	24	Q5R336	4.6	pdb11N81IA Chain A, Crystal Structure Of Pfg27 From <i>Plasmodium Falciparum</i>	1E-105		1.1

tr Q8I5P5 Q8I5P5_PLAF7 Glycerol-3-phosphate dehydrogenase, <b>putative</b>	103.0	25	Q8N335	1E-77	pdb 1YJ8 C Chain C, Initial Structural Analysis Of <b>Plasmodium Falciparum</b> Glycerol-3-Phosphate Dehydrogenase	1E-180	4420_all_target_protein.fasta Glycerol-3-phosphate dehydrogenase [NAD+], cytoplasmic (DB00157)	5E-75
tr Q8I377 Q8I377_PLAF7 ATP-dependent heat shock protein, <b>putative</b>	102.3	26	CLPX_HUMAN	2E-09	pdb 1D00 F Chain F, Orthorhombic Crystal Form Of Heat Shock Locus U (Hslu) From Escherichia Coli	1E-111	2254_all_target_protein.fasta ATP-dependent hsl protease ATP-binding subunit hslU (DB04395)	1E-111
tr Q8I4Y0 Q8I4Y0_PLAF7 Kinesin-like protein, <b>putative</b>	99.8	27	Q5T7B7	6E-81	pdb 1RY6 A Chain A, Crystal Structure Of Internal Kinesin Motor Domain	1E-180	1827_all_target_protein.fasta Kinesin-like protein KIF2C (DB03431; DB04395)	3E-79
tr Q8I3W2 Q8I3W2_PLAF7 Ribose 5-phosphate epimerase, <b>putative</b>	97.3	28	RPIA_HUMAN	2E-28	pdb 2F8M B Chain B, Ribose 5-Phosphate Isomerase From <b>Plasmodium Falciparum</b>	1E-125	180_all_target_protein.fasta Ribose-5-phosphate isomerase A (DB01756)	1E-29
tr Q76NM5 Q76NM5_PLAF7 Erythrocyte binding antigen 140	97.3	29	REST_HUMAN	9	pdb 1ZRO B Chain B, Crystal Structure Of Eba-175 Region Ii (Rii) Crystallized In The Presence Of (Alpha)2,3-Sialyllactose	5E-97	359_all_target_protein.fasta <b>NADH dehydrogenase</b> [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial (DB00157)	3.2
tr Q6LEZ4 Q6LEZ4_PLAF7 Putative 6-pyruvoyl tetrahydropterin synthase (6-pyruvoyl tetrahydropterin synthase, <b>putative</b> )	96.1	30	BRD7_HUMAN	0.4	pdb 1Y13 C Chain C, Structural Analysis Of <b>Plasmodium Falciparum</b> 6-Pyruvoyl Tetrahydropterin Synthase (Ptps)	3E-97	52_all_target_protein.fasta 6-pyruvoyl tetrahydrobiopterin synthase (DB03886)	0.13
sp Q8ILQ7 GST_PLAF7 Glutathione S-transferase	93.9	31	PTGD2_HUMAN	7E-18	pdb 2AAW C Chain C, Studies On Ligand Binding And Enzyme Inhibition Of <b>Plasmodium Falciparum</b> Glutathione S-Transferase	1E-111	2834_all_target_protein.fasta <b>Glutathione S-transferase</b> (DB01942; DB04132)	1E-112
tr Q8IJ7 Q8IJ7_PLAF7 Deoxyribose-phosphate aldolase, <b>putative</b>	92.6	32	DEOC_HUMAN	4E-22	pdb 2A4A B Chain B, Deoxyribose-Phosphate Aldolase From P. Yoelii	1E-114	4149_all_target_protein.fasta Deoxyribose-phosphate aldolase (DB04087)	4E-32
tr Q8ILQ2 Q8ILQ2_PLAF7 Glutathione reductase	91.3	33	GSHR_HUMAN	2E-89	pdb 1ONF A Chain A, Crystal Structure Of <b>Plasmodium Falciparum</b> Glutathione Reductase	1E-180	1508_all_target_protein.fasta <b>Glutathione reductase</b> (DB03147)	1E-180
sp Q7KQM0 TPIS_PLAF7 Triosephosphate isomerase	87.3	34	Q6FHP9	2E-58	pdb 1O5X B Chain B, <b>Plasmodium Falciparum</b> Tim Complexed To 2-Phosphoglycerate	1E-145	3437_all_target_protein.fasta <b>Triosephosphate isomerase</b> (DB01709; DB01779; DB02515; DB02726; DB02951; DB04510)	1E-146
tr Q8I372 Q8I372_PLAF7 Formylmethionine deformylase, <b>putative</b>	85.6	35	DEFM_HUMAN	4E-16	pdb 1RL4 B Chain B, <b>Plasmodium Falciparum</b> Peptide Deformylase Complex With Inhibitor	1E-101	2132_all_target_protein.fasta Formylmethionine <b>deformylase</b> , putative (DB02625; DB03648)	1E-139
tr Q8I6T4 Q8I6T4_PLAF7 Beta-hydroxyacyl-acp dehydratase	84.4	36	TNFL6_HUMAN	4.8	pdb 1Z6B F Chain F, Crystal Structure Of <b>Plasmodium Falciparum</b> Fabz At 2.1 A	2E-84	1863_all_target_protein.fasta 3-hydroxydecanoyl-[acyl-carrier-protein] dehydratase (DB03813)	0.12
tr Q3V7I1 Q3V7I1_PLAF7 <b>Putative</b> pyridoxine biosynthetic enzyme pdx1 homologue (Pyridoxine biosynthetic enzyme pdx1 homologue, <b>putative</b> )	83.4	37	GOGB1_HUMAN	0.24	pdb 1ZNN F Chain F, Structure Of The Synthase Subunit Of Plp Synthase	1E-84	1988_all_target_protein.fasta Modification methylase RsrI (DB01752; DB01910; DB02282)	0.92
tr O77330 O77330_PLAF7 Asparagine synthetase, <b>putative</b>	82.7	38	ASNS_HUMAN	5E-80	pdb 1CT9 D Chain D, Crystal Structure Of Asparagine Synthetase B From Escherichia Coli	1E-162	2840_all_target_protein.fasta Asparagine synthetase [glutamine-hydrolyzing] (DB00128; DB00130; DB00142; DB00171; DB00174)	7E-81
tr Q8I5L3 Q8I5L3_PLAF7 D-ribose-5-phosphate 3-epimerase, <b>putative</b>	82.5	39	RPE_HUMAN	3E-52	pdb 1TQX B Chain B, Crystal Structure Of PfaI009167 A Putative D-Ribulose 5- Phosphate 3-Epimerase From <b>P.Falciparum</b>	1E-134	1605_all_target_protein.fasta Delta 1-pyrroline-5-carboxylate synthetase (DB00142)	0.43

tr Q8I1R6 Q8I1R6_PLAF7 Bifunctional dihydrofolate reductase-thymidylate synthase	81.9	40	TYSY_HUMAN	8E-99	pdb1J3KID Chain D, Quadruple Mutant (N51i+c59r+s108n+i164l) <b>Plasmodium Falciparum</b> Dihydrofolate Reductase- Thymidylate Synthase (Pfdhfr-Ts) Complexed With Wr99210, Nadph, And Dump	1E-180	1991_all_target_protein.fasta <b>Bifunctional dihydrofolate reductase- thymidylate synthase (DB020205; DB01131)</b> 4516_all_target_protein.fasta Hypoxanthine-guanine-xanthine <b>phosphoribosyltransferase</b> (DB02075; DB02212)	1E-180
tr Q8IJS1 Q8IJS1_PLAF7 Hypoxanthine phosphoribosyltransferase	81.0	41	HPRT_HUMAN	9E-54	pdb11CJBID Chain D, <b>Malarial</b> Purine Phosphoribosyltransferase pdb11XIYIB Chain B, Crystal Structure Of <b>Plasmodium Falciparum</b> Antioxidant Protein (1- Cys Peroxiredoxin)	1E-134	1225_all_target_protein.fasta <b>Peroxiredoxin</b> (DB03661) 1014_all_target_protein.fasta <b>Adenylosuccinate synthetase</b> (DB02109; DB03510; DB04315)	1E-134
tr Q8IBG7 Q8IBG7_PLAF7 Antioxidant protein, <b>putative</b>	80.0	42	PRDX5_HUMAN	2E-14	pdb11P9BIA Chain A, Structure Of Fully Ligated Adenylosuccinate Synthetase From <b>Plasmodium Falciparum</b>	2E-94	1012_all_target_protein.fasta <b>Fructose-bisphosphate aldolase A</b> (DB02512; DB04326; DB04733)	6E-97
tr Q8IDF6 Q8IDF6_PLAF7 Adenylosuccinate synthetase	80.0	43	PURA2_HUMAN	1E-100	pdb11A5CIB Chain B, Fructose-1,6- Bisphosphate Aldolase From <b>Plasmodium Falciparum</b>	1E-180	2909_all_target_protein.fasta <b>Deoxyuridine 5'-triphosphate nucleotidohydrolase, putative</b> (DB04685)	1E-180
sp Q7KQL9 ALF_PLAF7 Fructose-bisphosphate aldolase	78.0	44	ALDOC_HUMAN	1E-102	pdb11VYQIC Chain C, Novel Inhibitors Of <b>Plasmodium Falciparum</b> Dutpase Provide A Platform For Anti-Malarial Drug Design	1E-180	460_all_target_protein.fasta Guanylate kinase (DB01972; DB03431)	1E-97
tr Q8II92 Q8II92_PLAF7 Deoxyuridine 5'-triphosphate nucleotidohydrolase, <b>putative</b>	76.4	45	DUT_HUMAN	7E-08	pdb11Z6GIA Chain A, Crystal Structure Of Guanylate Kinase From <b>Plasmodium Falciparum</b>	3E-84	137_all_target_protein.fasta Retinoic acid receptor beta (DB02877)	2E-84
tr Q8I2M1 Q8I2M1_PLAF7 Guanylate kinase, <b>putative</b>	75.3	46	Q5T435	2E-32	pdb11QUMIA Chain A, Crystal Structure Of Escherichia Coli Endonuclease Iv In Complex With Damaged Dna	1E-107	2730_all_target_protein.fasta <b>1- deoxy-D-xylulose 5-phosphate reductoisomerase</b> (DB04184)	1E-35
tr Q8IE02 Q8IE02_PLAF7 Apurinic/apurimidinic endonuclease Apn1	74.9	47	RARB_HUMAN	1.5	pdb11R0LID Chain D, 1-Deoxy-D-Xylulose 5- Phosphate Reductoisomerase From Zymomonas Mobilis In Complex With Nadph	2E-75	349_all_target_protein.fasta Isovaleryl-CoA dehydrogenase, mitochondrial (DB03147; DB04036)	0.18
tr Q8IKG4 Q8IKG4_PLAF7 1- deoxy-D-xylulose 5-phosphate reductoisomerase	73.3	48	No hit found	1000	pdb11ZSOIB Chain B, Hypothetical Protein From <b>Plasmodium Falciparum</b>	5E-71	568_all_target_protein.fasta <b>Superoxide dismutase [Mn], mitochondrial (DB04436)</b>	9E-72
tr Q8IDI8 Q8IDI8_PLAF7 <b>Putative uncharacterized</b> protein MAL13P1.257	72.5	49	Q9NWX4	3E-14	pdb12AWPIB Chain B, Crystal Structure Of <b>Plasmodium</b> Knowlesi Structure Of Iron Super- Oxide Dismutase	1E-86		0.25
sp Q8IAY6 SODF_PLAF7 Superoxide dismutase [Fe]	70.6	50	Q5TCM1	4E-38		1E-108		7E-39