

Supporting information

Title of manuscript:

Bioinformatic and experimental fishing for artemisinin-interacting proteins from human nasopharyngeal cancer cells

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Supplementary Table I:

Top 200 proteins interacting with artemisinin scored by AutoDock

PDB-ID (+Chain)	SCORE	UNIPROT ID	UNIPROT LINK	DESCRIPTION (Uniprot or PDB)
1HDP	-14,43	PO2F2_HUMAN	uniprot	POU domain, class 2, transcription factor 2
1BV8	-13,7	A2MG_HUMAN	uniprot	Alpha-2-macroglobulin
2FLR_2	-12,64	FA7_HUMAN	uniprot	Coagulation factor VII
2CLC_1	-12,6	RASH_HUMAN	uniprot	GTPase HRas
2CL7_1	-12,44	RASH_HUMAN	uniprot	GTPase HRas
10PG_2	-11,7		uniprot	Crystal structure of the OPG2 Fab. An antireceptor antibody that mimics an RGD cell adhesion site
2CLS_1	-11,59	RND1_HUMAN	uniprot	Rho-related GTP-binding protein Rho6
2CLS_2	-11,57	RND1_HUMAN	uniprot	Rho-related GTP-binding protein Rho6
2REX_4	-11,55	PLXB1_HUMAN	uniprot	Plexin-B1
2EVW_1	-11,54	RASH_HUMAN	uniprot	GTPase HRas
1L3K_1	-11,53	ROA1_HUMAN	uniprot	Heterogeneous nuclear ribonucleoprotein A1
1Z3N_1	-11,47	ALDR_HUMAN	uniprot	Aldose reductase
1NVW_1	-11,41	RASH_HUMAN	uniprot	GTPase HRas
1M9J_2	-11,23	NOS3_HUMAN	uniprot	Nitric oxide synthase, endothelial
2RGC	-11,14	RASH_HUMAN	uniprot	GTPase HRas
2RGE	-11,12	RASH_HUMAN	uniprot	GTPase HRas
1NVU_1	-11,11	RASH_HUMAN	uniprot	GTPase HRas
1US0_1	-11,09	ALDR_HUMAN	uniprot	Aldose reductase
1EFH_2	-11,08	ST2A1_HUMAN	uniprot	Bile salt sulfotransferase
1Q22_1	-11,08	ST2B1_HUMAN	uniprot	Sulfotransferase family cytosolic 2B member 1
2BZG_1	-11,07	TPMT_HUMAN	uniprot	Thiopurine S-methyltransferase
1NVV_1	-11,06	RASH_HUMAN	uniprot	GTPase HRas
1Q20_1	-11,05	ST2B1_HUMAN	uniprot	Sulfotransferase family cytosolic 2B member 1
2D06_1	-11,05	ST1A1_HUMAN	uniprot	Sulfotransferase 1A1
1K8R_1	-11,04	BYR2_SCHPO	uniprot	Protein kinase byr2
1C1Y_1	-11,01	RAF1_HUMAN	uniprot	RAF proto-oncogene serine/threonine-protein kinase
2H57_3	-11,01	ARL6_HUMAN	uniprot	ADP-ribosylation factor-like protein 6
1NVX_1	-11	RASH_HUMAN	uniprot	GTPase HRas
2Z5F_1	-10,99	ST1B1_HUMAN	uniprot	Sulfotransferase family cytosolic 1B member 1
1XRJ_2	-10,98	UCK2_HUMAN	uniprot	Uridine-cytidine kinase 2
1HY3_2	-10,96	ST1E1_HUMAN	uniprot	Estrogen sulfotransferase
1G3M_2	-10,95	ST1E1_HUMAN	uniprot	Estrogen sulfotransferase
1S3X_1	-10,94	HSP71_HUMAN	uniprot	Heat shock 70 kDa protein 1
2A3R_1	-10,94	ST1A3_HUMAN	uniprot	Sulfotransferase 1A3/1A4

		N		
2E8A	-10,93	HSP71_HUMA N	uniprot	Heat shock 70 kDa protein 1
2GWH_2	-10,92	ST1C4_HUMA N	uniprot	Sulfotransferase 1C4
2PFH_1	-10,92	ALDR_HUMAN	uniprot	Aldose reductase
1ZC3_1	-10,91	EXOC8_RAT	uniprot	Exocyst complex component 8
1KSH_1	-10,9	ARL2_MOUSE	uniprot	ADP-ribosylation factor-like protein 2
3C0Y_3	-10,9	HDAC7_HUMA N	uniprot	Histone deacetylase 7
2GWH_1	-10,89	ST1C4_HUMA N	uniprot	Sulfotransferase 1C4
2UZI_3	-10,88	RASH_HUMAN	uniprot	GTPase HRas
3BH7_1	-10,88	ARL3_MOUSE	uniprot	ADP-ribosylation factor-like protein 3
1EFH_1	-10,87	ST2A1_HUMA N	uniprot	Bile salt sulfotransferase
2OW2_2	-10,86	MMP9_HUMA N	uniprot	Matrix metalloproteinase-9
1KSJ_1	-10,84	ARL2_MOUSE	uniprot	ADP-ribosylation factor-like protein 2
3RAP_1	-10,83	RAP2A_HUMA N	uniprot	Ras-related protein Rap-2a
1HE8_2	-10,82	PK3CG_HUMA N	uniprot	Phosphatidylinositol-4,5-bisphosphate 3-kinase catalytic subunit gamma isoform
1KT8_2	-10,79	BCAT2_HUMA N	uniprot	Branched-chain-amino-acid aminotransferase, mitochondrial
1Q1Q_1	-10,77	ST2B1_HUMA N	uniprot	Sulfotransferase family cytosolic 2B member 1
2E9S_1	-10,77	RAB6B_HUMA N	uniprot	Ras-related protein Rab-6B
2H57_1	-10,74	ARL6_HUMAN	uniprot	ADP-ribosylation factor-like protein 6
2H57_2	-10,74	ARL6_HUMAN	uniprot	ADP-ribosylation factor-like protein 6
2CL6_1	-10,73	RASH_HUMAN	uniprot	GTPase HRas
1WMA_1	-10,72	CBR1_HUMAN	uniprot	Carbonyl reductase [NADPH] 1
2GIL_1	-10,72	RAB6A_HUMA N	uniprot	Ras-related protein Rab-6A
1LS6_1	-10,71	ST1A1_HUMA N	uniprot	Sulfotransferase 1A1
2PRL	-10,7	PYRD_HUMAN	uniprot	Dihydroorotate dehydrogenase, mitochondrial
1ZTQ_3	-10,69	MMP13_HUMA N	uniprot	Collagenase 3
2REO	-10,69	ST1C3_HUMA N	uniprot	Putative sulfotransferase 1C3
1M9K_2	-10,68	NOS3_HUMAN	uniprot	Nitric oxide synthase, endothelial
2FV5_1	-10,68	ADA17_HUMA N	uniprot	ADAM 17
1Z08_1	-10,67	RAB21_HUMA N	uniprot	Ras-related protein Rab-21
2D39_1	-10,67	FCN1_HUMAN	uniprot	Ficolin-1
3BHV_2	-10,67	CCNA2_BOVIN	uniprot	Cyclin-A2
10GU_4	-10,66	CCNA2_HUMA N	uniprot	Cyclin-A2
2CLD_1	-10,66	RASH_HUMAN	uniprot	GTPase HRas
1XD2_1	-10,65	RASH_HUMAN	uniprot	GTPase HRas
2OW0_	-10,65	MMP9_HUMA	uniprot	Matrix metalloproteinase-9

2		N		
3CKL_1	-10,63	ST1B1_HUMA N	uniprot	Sulfotransferase family cytosolic 1B member 1
1Z08_2	-10,62	RAB21_HUMA N	uniprot	Ras-related protein Rab-21
2FGB_1	-10,61	AK1C3_HUMA N	uniprot	Aldo-keto reductase family 1 member C3
10IU_2	-10,6	CCNA2_HUMA N	uniprot	Cyclin-A2
1RMZ_1	-10,6	MMP12_HUMA N	uniprot	Macrophage metalloelastase
1YZQ_1	-10,6	RAB6A_HUMA N	uniprot	Ras-related protein Rab-6A
10GU_2	-10,59	CCNA2_HUMA N	uniprot	Cyclin-A2
1UEA_1	-10,59	MMP3_HUMA N	uniprot	Stromelysin-1
20VZ_1	-10,59	MMP9_HUMA N	uniprot	Matrix metalloproteinase-9
1UAD_2	-10,58	EXOC2_RAT	uniprot	Exocyst complex component 2
1S1P_1	-10,56	AK1C3_HUMA N	uniprot	Aldo-keto reductase family 1 member C3
1S1R_1	-10,55	AK1C3_HUMA N	uniprot	Aldo-keto reductase family 1 member C3
1ZQ5_1	-10,55	AK1C3_HUMA N	uniprot	Aldo-keto reductase family 1 member C3
3CKL_2	-10,55	ST1B1_HUMA N	uniprot	Sulfotransferase family cytosolic 1B member 1
1OIX_1	-10,54	RB11A_HUMA N	uniprot	Ras-related protein Rab-11A
3C0Z_3	-10,54	HDAC7_HUMA N	uniprot	Histone deacetylase 7
1KTA_1	-10,53	BCAT2_HUMA N	uniprot	Branched-chain-amino-acid aminotransferase, mitochondrial
1QIA_1	-10,53	MMP3_HUMA N	uniprot	Stromelysin-1
1A8F_1	-10,52	TRFE_HUMAN	uniprot	Serotransferrin
2Q0Z_1	-10,52	U520_HUMAN	uniprot	U5 small nuclear ribonucleoprotein 200 kDa helicase
9JDW_1	-10,52	GATM_HUMAN	uniprot	Glycine amidinotransferase, mitochondrial
1YBW_1	-10,51	HGFA_HUMAN	uniprot	Hepatocyte growth factor activator
2EXX_2	-10,51	NMRL1_HUMA N	uniprot	NmrA-like family domain-containing protein 1
121P_1	-10,5	RASH_HUMAN	uniprot	GTPase HRas
20W0_1	-10,5	MMP9_HUMA N	uniprot	Matrix metalloproteinase-9
1G4G	-10,49	APOH_HUMAN	uniprot	Beta-2-glycoprotein 1
2I7T_1	-10,49	CPSF3_HUMA N	uniprot	Cleavage and polyadenylation specificity factor subunit 3
2ATH_1	-10,47	PPARG_HUMA N	uniprot	Peroxisome proliferator-activated receptor gamma
2COI_1	-10,47	BCAT1_HUMA N	uniprot	Branched-chain-amino-acid aminotransferase, cytosolic
2QME_1	-10,47	RAC3_HUMAN	uniprot	Ras-related C3 botulinum toxin substrate 3
421P_1	-10,47	RASH_HUMAN	uniprot	GTPase HRas

1XF0_1	-10,46	AK1C3_HUMA N	uniprot	Aldo-keto reductase family 1 member C3
1YRY_1	-10,46	PNPH_HUMAN	uniprot	Purine nucleoside phosphorylase
1Q1Z_1	-10,44	ST2B1_HUMA N	uniprot	Sulfotransferase family cytosolic 2B member 1
1S2C_1	-10,43	AK1C3_HUMA N	uniprot	Aldo-keto reductase family 1 member C3
1SUV_2	-10,43	TFR1_HUMAN	uniprot	Transferrin receptor protein 1
2B9R_2	-10,42	CCNB1_HUMA N	uniprot	G2/mitotic-specific cyclin-B1
2F38_1	-10,42	AK1C3_HUMA N	uniprot	Aldo-keto reductase family 1 member C3
2OW1_2	-10,42	MMP9_HUMA N	uniprot	Matrix metalloproteinase-9
521P_1	-10,42	RASH_HUMAN	uniprot	GTPase HRas
1BZY_1	-10,41	HPRT_HUMAN	uniprot	Hypoxanthine-guanine phosphoribosyltransferase
1DVA_1	-10,41	FA7_HUMAN	uniprot	Coagulation factor VII
1YZT_2	-10,41	RAB21_HUMA N	uniprot	Ras-related protein Rab-21
1RYO_1	-10,4	TRFE_HUMAN	uniprot	Serotransferrin
2C5L_1	-10,4	PLCE1_HUMA N	uniprot	1-phosphatidylinositol-4,5-bisphosphate phosphodiesterase epsilon-1
3BHV_4	-10,4	CCNA2_BOVIN	uniprot	Cyclin-A2
1E96_1	-10,39	NCF2_HUMAN	uniprot	Neutrophil cytosol factor 2
1JST_2	-10,39	CCNA2_HUMA N	uniprot	Cyclin-A2
1ZD9_1	-10,38	ARL8A_HUMA N	uniprot	ADP-ribosylation factor-like protein 8A
2HD5_1	-10,38	UBIQ_BOVIN	uniprot	Ubiquitin
1G3M_1	-10,37	ST1E1_HUMA N	uniprot	Estrogen sulfotransferase
1M9K_1	-10,36	NOS3_HUMAN	uniprot	Nitric oxide synthase, endothelial
3BFX_2	-10,35	ST1C2_HUMA N	uniprot	Sulfotransferase 1C2
1AGP_1	-10,34	RASH_HUMAN	uniprot	GTPase HRas
2DVQ_1	-10,34	BRD2_HUMAN	uniprot	Bromodomain-containing protein 2
2Z5F_2	-10,34	ST1B1_HUMA N	uniprot	Sulfotransferase family cytosolic 1B member 1
1N6K_1	-10,33	RAB5A_HUMA N	uniprot	Ras-related protein Rab-5A
1X9Q_1	-10,33		uniprot	4m5.3 anti-fluorescein single chain antibody fragment
2CE2_1	-10,33	RASH_HUMAN	uniprot	GTPase HRas
2Q8E_2	-10,33	JHD3A_HUMA N	uniprot	JmjC domain-containing histone demethylation protein 3A
1EK5_1	-10,32	GALE_HUMAN	uniprot	UDP-glucose 4-epimerase
2BWG_3	-10,32	GMPR1_HUMA N	uniprot	GMP reductase 1
2FFQ_1	-10,32	RAB6B_HUMA N	uniprot	Ras-related protein Rab-6B
1HE1_3	-10,31	RAC1_HUMAN	uniprot	Ras-related C3 botulinum toxin substrate 1
1WNT_1	-10,31	DCXR_HUMAN	uniprot	L-xylulose reductase
1YZU_1	-10,31	RAB21_HUMA N	uniprot	Ras-related protein Rab-21

2DVR_1	-10,31	BRD2_HUMAN	uniprot	Bromodomain-containing protein 2
2DVS_1	-10,31	BRD2_HUMAN	uniprot	Bromodomain-containing protein 2
1H28_2	-10,3	CCNA2_HUMAN	uniprot	Cyclin-A2
1HE1_4	-10,3	RAC1_HUMAN	uniprot	Ras-related C3 botulinum toxin substrate 1
1T91_1	-10,3	RAB7A_HUMAN	uniprot	Ras-related protein Rab-7a
1ZW6_1	-10,3	RASH_HUMAN	uniprot	GTPase HRas
2RBE_2	-10,3		uniprot	The discovery of 2-anilinothiazolones as 11beta-HSD1 inhibitors
1P2V_1	-10,29	RASH_HUMAN	uniprot	GTPase HRas
1R3W_1	-10,29	DCUP_HUMAN	uniprot	Uroporphyrinogen decarboxylase
1YZT_1	-10,29	RAB21_HUMAN	uniprot	Ras-related protein Rab-21
2RBE_4	-10,29		uniprot	The discovery of 2-anilinothiazolones as 11beta-HSD1 inhibitors
1ERR_1	-10,28	ESR1_HUMAN	uniprot	Estrogen receptor
1NCV	-10,28	CCL7_HUMAN	uniprot	C-C motif chemokine 7
3BCJ	-10,28	ALDR_HUMAN	uniprot	Aldose reductase
1GUA_1	-10,27	RAF1_HUMAN	uniprot	RAF proto-oncogene serine/threonine-protein kinase
2FXK_1	-10,27	H2AY_HUMAN	uniprot	Core histone macro-H2A.1
1I3M_2	-10,26	GALE_HUMAN	uniprot	UDP-glucose 4-epimerase
1JDX_1	-10,26	GATM_HUMAN	uniprot	Glycine amidinotransferase, mitochondrial
1QMB_1	-10,26	A1AT_HUMAN	uniprot	Alpha-1-antitrypsin
2Q8E_1	-10,25	JHD3A_HUMAN	uniprot	JmjC domain-containing histone demethylation protein 3A
2RBE_3	-10,25		uniprot	The discovery of 2-anilinothiazolones as 11beta-HSD1 inhibitors
1ZMD_3	-10,24	DLDH_HUMAN	uniprot	Dihydrolipoyl dehydrogenase, mitochondrial
2OV2_4	-10,24	PAK4_HUMAN	uniprot	Serine/threonine-protein kinase PAK 4
2RDW	-10,23	HAOX1_HUMAN	uniprot	Hydroxyacid oxidase 1
1JMO_2	-10,22	HEP2_HUMAN	uniprot	Heparin cofactor 2
1S2A_1	-10,22	AK1C3_HUMAN	uniprot	Aldo-keto reductase family 1 member C3
2BWG_2	-10,22	GMPR1_HUMAN	uniprot	GMP reductase 1
2OV2_3	-10,22	PAK4_HUMAN	uniprot	Serine/threonine-protein kinase PAK 4
2OW1_1	-10,22	MMP9_HUMAN	uniprot	Matrix metalloproteinase-9
2Q3F_1	-10,22	RRAGD_HUMAN	uniprot	Ras-related GTP-binding protein D
2BWG_1	-10,21	GMPR1_HUMAN	uniprot	GMP reductase 1
2IW8_2	-10,21	CCNA2_HUMAN	uniprot	Cyclin-A2
966C_1	-10,21	MMP1_HUMAN	uniprot	Interstitial collagenase
1N7W_1	-10,2	TRFE_HUMAN	uniprot	Serotransferrin
1PJ3_1	-10,2	MAOM_HUMAN	uniprot	NAD-dependent malic enzyme, mitochondrial
1Z28_1	-10,2	ST1A1_HUMAN	uniprot	Sulfotransferase 1A1

		N		
2E82_1	-10,2	OXDA_HUMAN	uniprot	D-amino-acid oxidase
2H8K	-10,2	ST1C3_HUMA N	uniprot	Putative sulfotransferase 1C3
5P21_1	-10,2	RASH_HUMAN	uniprot	GTPase HRas
20X0_2	-10,19	JHD3A_HUMA N	uniprot	JmjC domain-containing histone demethylation protein 3A
2REX_2	-10,19	PLXB1_HUMA N	uniprot	Plexin-B1
3BT1_2	-10,19	UPAR_HUMAN	uniprot	Urokinase plasminogen activator surface receptor
721P_1	-10,19	RASH_HUMAN	uniprot	GTPase HRas
8JDW_1	-10,19	GATM_HUMAN	uniprot	Glycine amidinotransferase, mitochondrial
1PWM_1	-10,18	ALDR_HUMAN	uniprot	Aldose reductase
1R4A_1	-10,18	ARL1_RAT	uniprot	ADP-ribosylation factor-like protein 1
2H4Z_2	-10,18	PMGE_HUMAN	uniprot	Bisphosphoglycerate mutase
2OV2_2	-10,17	PAK4_HUMAN	uniprot	Serine/threonine-protein kinase PAK 4
1RY8_1	-10,16	AK1C3_HUMA N	uniprot	Aldo-keto reductase family 1 member C3
1T5A_1	-10,16	KPYM_HUMAN	uniprot	Pyruvate kinase isozymes M1/M2
2DU8_1	-10,16	OXDA_HUMAN	uniprot	D-amino-acid oxidase
2FVL_1	-10,16	AK1C4_HUMA N	uniprot	Aldo-keto reductase family 1 member C4
2I40_4	-10,16	CCNA2_HUMA N	uniprot	Cyclin-A2
2OV2_1	-10,16	PAK4_HUMAN	uniprot	Serine/threonine-protein kinase PAK 4
2QXM_1	-10,16	ESR1_HUMAN	uniprot	Estrogen receptor
3BFX_1	-10,15	ST1C2_HUMA N	uniprot	Sulfotransferase 1C2
1A1M_1	-10,14	1B53_HUMAN	uniprot	HLA class I histocompatibility antigen, B-53 alpha chain
1EUB_1	-10,14	MMP13_HUMA N	uniprot	Collagenase 3
1FDU_2	-10,14	DHB1_HUMAN	uniprot	Estradiol 17-beta-dehydrogenase 1
1M9Q_1	-10,14	NOS3_HUMAN	uniprot	Nitric oxide synthase, endothelial
1RY0_1	-10,14	AK1C3_HUMA N	uniprot	Aldo-keto reductase family 1 member C3
1VYW_2	-10,13	CCNA2_HUMA N	uniprot	Cyclin-A2
1VYW_4	-10,13	CCNA2_HUMA N	uniprot	Cyclin-A2
1ZTQ_4	-10,13	MMP13_HUMA N	uniprot	Collagenase 3
2BPM_2	-10,13	CCNA2_HUMA N	uniprot	Cyclin-A2