

Table S1 PharmMapper predicted the potential target of IMB5043

Pharma Model	Uniprot	Num Feature	Fit	Norm Fit	z-score
2vwu	EPHB4	3	2.992	0.9973	1.557170
1klt	CMA1	3	2.891	0.9637	1.257850
1w8m	PPIA	3	2.804	0.9347	0.873965
1unh	CDK5R1	3	2.719	0.9064	0.666043
1pq9	NR1H2	3	2.660	0.8866	0.340896
1zfq	CA2	3	2.646	0.8820	0.501950
3fzk	HSPA8	3	2.512	0.8750	3.775610
1lbk	GSTP1	4	2.565	0.8550	-0.219390
1x97	AKR1B1	3	2.556	0.8522	0.189525
1ya8	CES1	3	2.539	0.8462	-0.062370
2ovm	PSR	3	2.520	0.8400	0.015955
1pmv	MAPK10	3	2.514	0.8381	-1.016890
1xlv	BCHE	3	2.401	0.8002	-0.297980
2ocf	ESR1	3	2.314	0.7715	-0.712880
2g01	MAPK8	4	2.975	0.7437	1.342630
2j5f	EGFR	4	2.963	0.7408	1.375120
2j38	F10	4	2.955	0.7387	1.361680
1csb	CTSB	4	2.926	0.7316	1.369560
2ywp	CHEK1	4	2.922	0.7305	1.367480
1zyj	MAPK14	4	2.890	0.7224	0.913300
2h8h	SRC	4	2.888	0.7221	1.131800
1t4v	F2	4	2.878	0.7195	1.204860
1vjy	TGFBFR1	4	2.877	0.7192	0.976537
2jdt	PRKACA	4	2.870	0.7175	1.073420
2fky	KIF11	4	2.860	0.7150	0.414080
1ld7	FNTA	4	2.858	0.7145	0.964029
1fm6	PPARG	4	2.857	0.7143	0.805510
1a8j	IGLV2-8	4	2.856	0.7139	1.113040
1bm6	MMP3	3	2.134	0.7113	-2.056310
1hak	ANXA5	4	2.818	0.7044	0.364556
5gal	LGALS7	4	2.811	0.7027	0.950854
3bgq	PIM1	4	2.803	0.7006	0.638211
1ckp	CDK2	4	2.800	0.6999	0.849128
1dic	CFD	4	2.773	0.6932	0.691180
1xur	MMP13	4	2.761	0.6902	0.751486
2rku	PLK1	4	2.726	0.6815	0.573903
2f6y	PTPN1	4	2.700	0.6751	0.408422
1q8m	TREM1	3	2.013	0.6709	-1.605910
2acl	RXRA	4	2.676	0.6690	0.254098
1i72	AMD1	4	2.641	0.6603	0.476442
3bmy	HSP90AA1	4	2.558	0.6395	-0.137710
1gcz	MIF	4	2.537	0.6343	-0.243880
1m4u	BMP7	4	2.490	0.6225	-0.383120
1waw	CHIT1	4	2.483	0.6208	-0.495040
1m51	PCK1	6	3.640	0.6066	1.911540
1t84	WAS	5	2.997	0.5995	0.768372
2bkz	CCNA2	4	2.390	0.5976	-0.824930
2bub	DPF4	5	2.934	0.5868	1.174390
1o6u	SEC14L2	4	2.930	0.5860	0.388318
2pe0	PDPK1	4	2.339	0.5847	-1.109360
2rfn	MET	5	2.916	0.5833	0.985443
1utt	MMP12	5	2.916	0.5832	0.998049
1bm7	TTR	5	2.915	0.5831	0.584805
1dmw	PAH	5	2.911	0.5823	0.873641
2bx8	ALB	5	2.905	0.5809	0.448916
3f0r	HDAC8	5	2.903	0.5807	0.821993
1mq0	CDA	5	2.902	0.5805	1.264040
3blr	CCNT1	5	2.899	0.5799	1.267240
1xbc	SYK	5	2.894	0.5788	0.841218
1e8z	PIK3CG	5	2.890	0.5780	0.879118
1yk7	CTSK	5	2.887	0.5774	1.112240
2v5z	MAOB	4	2.309	0.5772	-1.359750
1q5k	GSK3B	5	2.877	0.5754	0.887321
1zs0	MMP8	4	2.301	0.5753	-1.066700
3czz	HSD11B1	5	2.874	0.5747	0.243452
1fji	FGFR1	5	2.869	0.5738	1.043770
1a7a	AHCY	5	2.865	0.5729	0.635204
1ro6	PDE4B	5	2.856	0.5712	0.695739
1k59	ANG	4	2.282	0.5705	-2.274660
2rf5	KDR	5	2.846	0.5693	0.519896
1rfm	CASP3	5	2.816	0.5631	0.911917
1xo2	CDK6	5	2.809	0.5618	0.693440
1h1b	ELANE	6	3.368	0.5613	2.661000
1qyx	HSD17B1	5	2.807	0.5613	-0.092020
1hkc	HK1	5	2.805	0.5610	0.603752
1wck	PARP1	5	2.796	0.5591	0.317162
2aa5	NR3C2	5	2.785	0.5570	0.125262
1xor	PDE4D	5	2.763	0.5525	0.436568
1snu	ITK	5	2.761	0.5521	0.295818
1wma	CBR1	5	2.747	0.5494	0.400065
2iku	REN	5	2.740	0.5481	0.384537
3dy6	PPARD	4	2.166	0.5416	-2.227980
1a5h	PLAT	5	2.698	0.5396	0.294951
1mrq	AKR1C1	5	2.695	0.5390	-0.050390
2opy	XIAP	5	2.682	0.5363	0.430801
1xil	SOD2	5	2.653	0.5305	-0.022190
1oec	FGFR2	5	2.650	0.5299	-0.448400
2shp	PTPN11	5	2.629	0.5257	-0.778640
2j7x	Esr2	4	2.089	0.5223	-1.740060
1d3h	DHODH	6	3.105	0.5175	1.485580
1og5	CYP2C9	6	3.078	0.5130	1.345780
1ov4	SULT2A1	5	2.557	0.5113	-1.155170
2q6c	HMGCR	5	2.551	0.5103	-0.618360
1ry8	AKR1C3	5	2.537	0.5074	-0.000420
1v45	PNP	4	2.016	0.5041	-1.907830
1wjj	ISG20	5	2.513	0.5026	-1.090640
1ju6	TYMS	6	2.999	0.4998	1.294170
1pl6	SORD	5	2.496	0.4991	-1.178550
2i6b	ADK	6	2.994	0.4990	0.465112
1xvp	NR1I3	6	2.989	0.4981	0.784598
2a8h	ADAM17	6	2.985	0.4974	1.351880
1t4e	MDM2	6	2.985	0.4974	0.483892
1i7g	PPARA	6	2.969	0.4949	0.838031
1uhl	NR1H3	6	2.963	0.4938	0.711399
1dxo	NQO1	6	2.949	0.4914	0.774603
1wda	PADI4	6	2.926	0.4876	0.636173
1he2	BLVRB	6	2.923	0.4872	0.781299
1sgx	TGM3	6	2.907	0.4845	0.804152
1udt	PDE5A	6	2.897	0.4828	1.095870
3bbt	ERBB4	6	2.893	0.4821	0.524574
1qpd	LCK	6	2.891	0.4819	0.290348
1gse	GSTA1	6	2.880	0.4800	0.191945
1so2	PDE3B	5	2.398	0.4795	-1.374620
1vj5	EPHX2	5	2.396	0.4791	-1.334670
1tw6	BIRC7	6	2.870	0.4783	1.064030
1g8i	NCS1	5	2.385	0.4770	-0.653690
1s9p	ESRRG	6	2.852	0.4753	0.328626
1yvj	JAK3	6	2.851	0.4752	0.195259
3d7t	CSK	6	2.848	0.4746	0.511070
1lzj	ABO	6	2.821	0.4702	0.869365
2bu5	PDK2	6	2.819	0.4698	-0.117110
1isg	BST1	6	2.805	0.4674	0.268095
1xq3	AR	6	2.800	0.4666	-0.070430
1v84	B3GAT1	6	2.797	0.4662	0.636792
1hlc	LGALS2	6	2.795	0.4658	0.502474
1tjj	GM2A	6	2.794	0.4656	0.409846
1t2f	LDHB	5	2.326	0.4652	-1.964510
1qab	RBP4	6	2.789	0.4649	-0.00097
1lhn	SHBG	6	2.788	0.4646	-0.253860
1hti	TP11	6	2.779	0.4632	-0.034190
2gv7	ST14	6	2.773	0.4621	0.771876
1u4l	CCL5	6	2.770	0.4616	0.444328
2rjp	ADAMTS4	6	2.768	0.4613	0.784954
1mc5	ADH5	7	3.222	0.4602	0.390058
2zdz	BACE1	6	2.745	0.4575	0.015963
1dhf	DHFR	6	2.724	0.4540	0.008036
1npz	CTSS	8	3.626	0.4532	3.112430
1nd5	ACP3	6	2.696	0.4493	-0.531670
2c30	PAK6	6	2.692	0.4487	-0.366080
1bj4	SHMT1	6	2.691	0.4485	0.0753820
3d2e	SSE1	6	2.686	0.4477	-0.149980
1dia	MTHFD1	6	2.660	0.4433	-0.160890
1o5f	HPN	5	2.187	0.4375	-1.585380
1sz7	TRAPPC3	6	2.603	0.4338	-0.781080
1ds6	RAC2	5	2.162	0.4325	-1.933100
2o9i	NR1I2	7	2.997	0.4281	0.433379
2f9b	F7	6	2.566	0.4276	-0.064730
1v2	HNF4G	7	2.990	0.4272	0.327442
1tou	FABP4	6	2.563	0.4272	-0.377120
1x9d	MAN1B1	7	2.990	0.4271	1.261230
2j4a	THR8	6	2.558	0.4263	-0.774190
1i3l	GALE	6	2.545	0.4241	-0.580260
1p62	DNK	7	2.958	0.4226	0.847544
2g8n	PNMT	5	2.109	0.4217	-2.326620
1fkg	FKBP1A	7	2.949	0.4213	0.557983
2ojj	MAPK1	7	2.938	0.4198	0.566768
1uzf	ACE	7	2.937	0.4196	0.051883
1dkf	RARA	8	3.353	0.4192	1.540910
1hmt	FABP3	7	2.933	0.4190	-0.026790
1x89	LCN2	7	2.933	0.4189	0.517698
1elv	C1S	6	2.504	0.4174	-0.91820
1m6d	CTSF	7	2.917	0.4168	0.828783
1mlw	TPH1	7	2.913	0.4162	0.331344
1p5j	SDS	7	2.911	0.4159	0.193997
1imx	IGF1	7	2.890	0.4128	0.238310
1iri	GPI	7	2.888	0.4126	-0.069080
2b7a	JAK2	7	2.887	0.4124	0.144131
1qcf	HCK	7	2.881	0.4115	0.025848
1s9j	MAP2K1	9	3.694	0.4105	1.521690
1db5	PLA2G2A	7	2.869	0.4098	0.435827
1qdd	REG1A	5	2.045	0.4091	-2.530050
1u59	ZAP70	7	2.859	0.4084	0.147385
1xoi	PYGL	7	2.859	0.4084	0.021603
1gkd	MMP9	7	2.855	0.4079	0.294069
1nav	THRA	7	2.853	0.4076	-0.140460
6fit	FHIT	6	2.440	0.4067	-0.828070
1lzi	ABO	7	2.846	0.4066	0.556223
1xjd	PRKCQ	7	2.842	0.4060	0.037746
1fcz	RARG	7	2.831	0.4045	0.054953
1irj	S100A9	7	2.820	0.4029	0.158981
1ljr	GSTT2B	7	2.818	0.4026	0.177918
1nxx	MAPKAPK2	7	2.818	0.4025	-0.034770
1uej	UCK2	6	2.411	0.4019	-1.418610
1m48	IL2	7	2.809	0.4013	0.107690
2zm3	IGF1R	6	2.406	0.4011	-1.153640
1osh	NR1H4	5	2.002	0.4004	-3.321590
1mt6	SETD7	7	2.790	0.3985	0.288641
1kjr	LGALS3	7	2.786	0.3981	0.767117
1t32	CTSG	7	2.782	0.3974	-0.104170
1gzu	NMNAT1	7	2.781	0.3973	-0.010640
1oiw	RAB11A	6	2.382	0.3971	-1.108350
1z57	CLK1	7	2.778	0.3969	0.069928
1q22	SULT2B1	7	2.775	0.3964	-0.339820
1dyt	RNASE3	6	2.347	0.3912	-2.05979
1r1h	MME	10	3.900	0.3900	1.184010
1o1v	FABP6	7	2.724	0.3891	-0.518710
1qh5	HAGH	7	2.668	0.3811	-0.409730
1tx4	ARHGAP1	6	2.276	0.3794	-1.354120
2fs9	TPSB2	8	3.032	0.3790	1.557400
1ne7	GNPDA2	7	2.644	0.3777	-0.427200
1nf7	IMPDH2	6	2.249	0.3748	-1.548990
1jqe	HNMT	8	2.997	0.3747	0.091572
2gqg	ABL1	8	2.995	0.3744	0.774761
1hrk	FECH	8	2.990	0.3737	0.399492
3bc3	CTSL	8			