

Table S3 Predicted target proteins that Xuan-Fu-Hua effective components potentially interact with

Ingredient	Effective component	Target protein	Probability
Inulae Flos (Xuan-Fu-Hua)	MOL000006	NOX4	1
	MOL000006	AKR1B1	1
	MOL000006	CDK5R1	1
	MOL000006	CDK5	1
	MOL000006	CDK1	1
	MOL000006	CCNB1	1
	MOL000006	CCNB2	1
	MOL000006	XDH	1
	MOL000006	MAOA	1
	MOL000006	FLT3	1
	MOL000006	CA2	1
	MOL000006	CCNB3	1
	MOL000006	ALOX5	1
	MOL000006	ADORA1	1
	MOL000006	CA7	1
	MOL000006	GLO1	1
	MOL000006	APP	1
	MOL000006	SYK	1
	MOL000006	GSK3B	1
	MOL000006	PARP1	1
	MOL000006	TTR	1
	MOL000006	MMP9	1
	MOL000006	CA12	1
	MOL000006	MMP2	1
	MOL000006	CA4	1
	MOL000006	MMP12	1
	MOL000006	CD38	1
	MOL000006	CYP1B1	1
	MOL000006	ABCG2	1
	MOL000006	AKR1B10	1
	MOL000006	TNKS2	1
	MOL000006	TNKS	1
	MOL000006	TOP1	1
	MOL000006	ARG1	1
	MOL000006	PTPRS	0.89772751
	MOL000006	ABCC1	0.65801974
	MOL000006	HSD17B1	0.65801974
	MOL000006	ACHE	0.62492123
	MOL000006	CDK6	0.62492123
	MOL000006	ABCB1	0.53450496

MOL000098	NOX4	1
MOL000098	AVPR2	1
MOL000098	AKR1B1	1
MOL000098	XDH	1
MOL000098	MAOA	1
MOL000098	IGF1R	1
MOL000098	FLT3	1
MOL000098	CYP19A1	1
MOL000098	EGFR	1
MOL000098	F2	1
MOL000098	CA2	1
MOL000098	PIM1	1
MOL000098	ALOX5	1
MOL000098	AURKB	1
MOL000098	DRD4	1
MOL000098	ADORA1	1
MOL000098	CA7	1
MOL000098	GLO1	1
MOL000098	MPO	1
MOL000098	PIK3R1	1
MOL000098	ADORA2A	1
MOL000098	DAPK1	1
MOL000098	PYGL	1
MOL000098	CA1	1
MOL000098	GSK3B	1
MOL000098	SRC	1
MOL000098	PTK2	1
MOL000098	HSD17B2	1
MOL000098	KDR	1
MOL000098	MMP13	1
MOL000098	MMP3	1
MOL000098	CA3	1
MOL000098	ALOX15	1
MOL000098	ABCC1	1
MOL000098	PLK1	1
MOL000098	CA6	1
MOL000098	CDK1	1
MOL000098	MMP9	1
MOL000098	CA12	1
MOL000098	MMP2	1
MOL000098	PKN1	1
MOL000098	CA14	1
MOL000098	CA9	1
MOL000098	CSNK2A1	1

MOL000098	ALOX12	1
MOL000098	MET	1
MOL000098	CA4	1
MOL000098	NEK2	1
MOL000098	CXCR1	1
MOL000098	CAMK2B	1
MOL000098	ALK	1
MOL000098	AKT1	1
MOL000098	ABCB1	1
MOL000098	NEK6	1
MOL000098	PLA2G1B	1
MOL000098	CA5A	1
MOL000098	BACE1	1
MOL000098	CYP1B1	1
MOL000098	AXL	1
MOL000098	ABCG2	1
MOL000098	NUAK1	1
MOL000098	AKR1C2	1
MOL000098	AKR1C1	1
MOL000098	AKR1C3	1
MOL000098	AKR1C4	1
MOL000098	CA13	1
MOL000098	AKR1A1	1
MOL000098	GPR35	0.99550367
MOL000098	SYK	0.70391175
MOL000098	MAPT	0.68028359
MOL000098	KDM4E	0.68028359
MOL000098	TOP2A	0.68028359
MOL000098	INSR	0.68028359
MOL000098	ACHE	0.68028359
MOL000098	MYLK	0.68028359
MOL000098	PIK3CG	0.68028359
MOL000098	APEX1	0.68028359
MOL000098	CDK5R1	0.56954598
MOL000098	CDK5	0.56954598
MOL000098	CDK1	0.56954598
MOL000098	CCNB1	0.56954598
MOL000098	CCNB2	0.56954598
MOL000098	CCNB3	0.56954598
MOL000098	ARG1	0.56954598
MOL000098	PTPRS	0.53806181
MOL000098	ESR2	0.53806181
MOL000098	MPG	0.53806181
MOL000098	SLC22A12	0.53806181

MOL000098	CDK6	0.52227789
MOL000098	CDK2	0.52227789
MOL000354	XDH	1
MOL000354	CA2	1
MOL000354	CA7	1
MOL000354	CA12	1
MOL000354	CA4	1
MOL000354	CYP1B1	1
MOL000358	AR	0.64764692
MOL000358	HMGCR	0.6143111
MOL000358	CYP51A1	0.6143111
MOL000358	NPC1L1	0.53100214
MOL000358	NR1H3	0.53100214
MOL000358	CYP19A1	0.53100214
MOL000422	NOX4	1
MOL000422	AKR1B1	1
MOL000422	XDH	1
MOL000422	TYR	1
MOL000422	FLT3	1
MOL000422	CA2	1
MOL000422	ALOX5	1
MOL000422	CA7	1
MOL000422	HSD17B2	1
MOL000422	ABCC1	1
MOL000422	HSD17B1	1
MOL000422	AHR	1
MOL000422	CA12	1
MOL000422	ESRRA	1
MOL000422	ABCB1	1
MOL000422	CYP1B1	1
MOL000422	ABCG2	1
MOL000422	ADORA1	0.79504726
MOL000422	CA4	0.79504726
MOL000422	ACHE	0.7684692
MOL000422	MAOA	0.65801974
MOL000422	GLO1	0.65801974
MOL000422	SYK	0.65801974
MOL000422	GSK3B	0.65801974
MOL000422	MMP9	0.65801974
MOL000422	MMP2	0.65801974
MOL000422	ALOX15	0.64978075
MOL000422	ALOX12	0.63332626
MOL000422	PTPRS	0.60844626
MOL000422	ADORA2A	0.5673019

	MOL000422	CDK5R1	0.50959976
	MOL000422	CDK5	0.50959976
	MOL000422	CDK1	0.50959976
	MOL000422	CCNB1	0.50959976
	MOL000422	CCNB2	0.50959976
	MOL000422	CCNB3	0.50959976
	MOL000422	ARG1	0.50959976
	MOL000422	GPR35	0.50153002
	MOL000422	ESR2	0.50153002
	MOL000422	DAPK1	0.50153002
	MOL000422	MPG	0.50153002
	MOL000422	SLC22A12	0.50153002
	MOL003044	ABCC1	1
	MOL003044	CYP1B1	1
	MOL004083	CYP1B1	1
	MOL004083	XDH	0.75150438
	MOL004083	CA2	0.72652335
	MOL004083	CA7	0.72652335
	MOL004083	CA12	0.72652335
	MOL004083	CA4	0.72652335
	MOL004083	ABCC1	0.53488748
	MOL004083	NOX4	1
	MOL004083	AKR1B1	0.61820168
	MOL004083	XDH	0.609848
	MOL004083	CYP1B1	0.50155586
Rubia Cordifolia	MOL000358	AR	0.64764692
(Qian-Cao)	MOL000358	HMGCR	0.6143111
	MOL000358	CYP51A1	0.6143111
	MOL000358	NPC1L1	0.53100214
	MOL000358	NR1H3	0.53100214
	MOL000358	CYP19A1	0.53100214
	MOL000359	AR	0.64764692
	MOL000359	HMGCR	0.6143111
	MOL000359	CYP51A1	0.6143111
	MOL000359	NPC1L1	0.53100214
	MOL000359	NR1H3	0.53100214
	MOL000359	CYP19A1	0.53100214
	MOL005869	AR	0.75594745
	MOL005869	CDC25A	0.53100214
	MOL006160	MCL1	1
	MOL006160	BCL2	1
	MOL006174	IDO1	1