

Table S1. Compounds and target used for network pharmacology analysis

No.	Compounds	Source of metabolites	Drug and vitiligo overlapping genes
C13	Calceolarioside B		PRKCA
C13	Calceolarioside B		MMP12
C13	Calceolarioside B		MMP2
C13	Calceolarioside B		AKR1B1
C13	Calceolarioside B		HSP90AA1
C13	Calceolarioside B		ADORA2A
C13	Calceolarioside B		MMP13
C13	Calceolarioside B		ADORA3
C13	Calceolarioside B		TNF
C13	Calceolarioside B		F3
C13	Calceolarioside B		SLC28A2
C13	Calceolarioside B		ALDH2
C13	Calceolarioside B		MMP7
C13	Calceolarioside B		MMP8
C13	Calceolarioside B		SLC28A3
C13	Calceolarioside B		IMPDH1
C13	Calceolarioside B		SLC29A1
C13	Calceolarioside B		MMP1
C13	Calceolarioside B		PARP1
C13	Calceolarioside B		APP
C13	Calceolarioside B		AKR1B10
C13	Calceolarioside B		MGMT
C13	Calceolarioside B		YARS
C13	Calceolarioside B		ANG
C13	Calceolarioside B		SRC
C13	Calceolarioside B		HMGCR
C13	Calceolarioside B		GSK3B
C13	Calceolarioside B		MMP13
C13	Calceolarioside B		YARS1
C13	Calceolarioside B		DHFR
C13	Calceolarioside B		HK1
C13	Calceolarioside B		HDAC8
C13	Calceolarioside B		RBP4
C13	Calceolarioside B		HEXB
C13	Calceolarioside B		ACP3
C13	Calceolarioside B		ABO
C13	Calceolarioside B		TGM3
C13	Calceolarioside B		GP1BA
C13	Calceolarioside B		GNPDA1
C13	Calceolarioside B		ELANE
C13	Calceolarioside B		HINT1
C13	Calceolarioside B		EPHA2
C13	Calceolarioside B		MMP16
C13	Calceolarioside B		CLEC4M
C13	Calceolarioside B		STAT1
C13	Calceolarioside B		ACAT1
C13	Calceolarioside B		GCDH
C13	Calceolarioside B		ARL5A
C13	Calceolarioside B		CD209
C13	Calceolarioside B		RND3
C13	Calceolarioside B		SELE
C24	Akebia saponin PJ1		GC
C24	Akebia saponin PJ1		SEC14L2
C24	Akebia saponin PJ1		PPARD
C24	Akebia saponin PJ1		WAS

C24	Akebia saponin PJ1	TTPA
C24	Akebia saponin PJ1	SORD
C24	Akebia saponin PJ1	PLA2G2A
C24	Akebia saponin PJ1	NR1H4
C24	Akebia saponin PJ1	FABP3
C24	Akebia saponin PJ1	ADH5
C24	Akebia saponin PJ1	ADK
C24	Akebia saponin PJ1	EPHB4
C24	Akebia saponin PJ1	TRAPPC3
C24	Akebia saponin PJ1	HSP90AA1
C24	Akebia saponin PJ1	SERPINA1
C24	Akebia saponin PJ1	FABP7
C24	Akebia saponin PJ1	PPARA
C24	Akebia saponin PJ1	MMP2
C24	Akebia saponin PJ1	MAP2K1
C24	Akebia saponin PJ1	NR1I2
C24	Akebia saponin PJ1	HMGCR
C24	Akebia saponin PJ1	RXRB
C24	Akebia saponin PJ1	MME
C24	Akebia saponin PJ1	MAPK12
C24	Akebia saponin PJ1	HGF
C24	Akebia saponin PJ1	INSR
C30	Akebia saponin E	PDE5A
C30	Akebia saponin E	GC
C30	Akebia saponin E	MMP13
C30	Akebia saponin E	PTPN1
C30	Akebia saponin E	EGFR
C30	Akebia saponin E	FNTA
C30	Akebia saponin E	PTPN11
C30	Akebia saponin E	HSD17B1
C30	Akebia saponin E	HSD11B1
C30	Akebia saponin E	HDAC8
C30	Akebia saponin E	TRAPPC3
C30	Akebia saponin E	ADH5
C30	Akebia saponin E	PDK2
C30	Akebia saponin E	FABP6
C30	Akebia saponin E	FABP7
C30	Akebia saponin E	HNF4G
C30	Akebia saponin E	IGF1
C30	Akebia saponin E	FABP3
C30	Akebia saponin E	THRA
C30	Akebia saponin E	RARG
C30	Akebia saponin E	CYP2C8
C30	Akebia saponin E	CTSG
C30	Akebia saponin E	FECH
C30	Akebia saponin E	PLEKHA4
C30	Akebia saponin E	HSP90AB1
C30	Akebia saponin E	RXRB
C30	Akebia saponin E	HGF
C30	Akebia saponin E	DCPS
C30	Akebia saponin E	CASP1
C30	Akebia saponin E	HSD11B2
C30	Akebia saponin E	HSD11B1
C31	Akebia saponin D	ANG
C31	Akebia saponin D	TTR
C31	Akebia saponin D	SULT2A1
C31	Akebia saponin D	AHCY
C31	Akebia saponin D	PTPN11

C31	Akebia saponin D	F10
C31	Akebia saponin D	CBR1
C31	Akebia saponin D	CES1
C31	Akebia saponin D	REN
C31	Akebia saponin D	LCK
C31	Akebia saponin D	THRA
C31	Akebia saponin D	RNASE3
C31	Akebia saponin D	FABP6
C31	Akebia saponin D	ABO
C31	Akebia saponin D	ACP3
C31	Akebia saponin D	HEXB
C31	Akebia saponin D	IGF1
C31	Akebia saponin D	BST1
C31	Akebia saponin D	TPH1
C31	Akebia saponin D	MMP2
C31	Akebia saponin D	S100A9
C31	Akebia saponin D	PRKCQ
C31	Akebia saponin D	ZAP70
C31	Akebia saponin D	ARG2
C31	Akebia saponin D	PDE5A
C31	Akebia saponin D	HRAS
C31	Akebia saponin D	STAT1
C31	Akebia saponin D	ATIC
C31	Akebia saponin D	APAF1
C31	Akebia saponin D	F11
C31	Akebia saponin D	ITPKA
C31	Akebia saponin D	UAP1
C31	Akebia saponin D	GMPR2
C42	Apigenin	FKBP1A
C42	Apigenin	VDR
C42	Apigenin	XDH
C42	Apigenin	MAOA
C42	Apigenin	ESR1
C42	Apigenin	ACHE
C42	Apigenin	PTGS2
C42	Apigenin	SYK
C42	Apigenin	PARP1
C42	Apigenin	ABCB1
C42	Apigenin	ALOX12
C42	Apigenin	MMP2
C42	Apigenin	ARG1
C42	Apigenin	ESRRA
C42	Apigenin	PFKFB3
C42	Apigenin	GRK6
C42	Apigenin	ALOX15
C42	Apigenin	TYR
C42	Apigenin	AHR
C42	Apigenin	CBR1
C42	Apigenin	AR
C42	Apigenin	BCHE
C42	Apigenin	CDK2
P1	Stachydrine	ACE
P1	Stachydrine	REN
P1	Stachydrine	SLC1A2
P1	Stachydrine	F2
P1	Stachydrine	ARG1
P2	Carasinaurone	MIF
P2	Carasinaurone	ACE

P2	Carasinaurone		ESR1
P3	Calycosin-7-O- β -D-glucoside		PAH
P3	Calycosin-7-O- β -D-glucoside		F2
P3	Calycosin-7-O- β -D-glucoside		CBR1
P3	Calycosin-7-O- β -D-glucoside		SOD2
P3	Calycosin-7-O- β -D-glucoside		AHCY
P3	Calycosin-7-O- β -D-glucoside		ABO
P3	Calycosin-7-O- β -D-glucoside		TNF
P3	Calycosin-7-O- β -D-glucoside		IL2
P3	Calycosin-7-O- β -D-glucoside		XDH
P4	Akebia saponin B		RORA
P4	Akebia saponin B		F2
P4	Akebia saponin B		DPP4
P4	Akebia saponin B		NR1H2
P4	Akebia saponin B		REN
M2		Calycosin-7-O- β -D-glucoside (C12)	PAH
M2		Calycosin-7-O- β -D-glucoside (C12)	DPP4
M2		Calycosin-7-O- β -D-glucoside (C12)	CCL5
M2		Calycosin-7-O- β -D-glucoside (C12)	ABO
M2		Calycosin-7-O- β -D-glucoside (C12)	PMS2
M5		Apigenin (C42)	CDK2
M5		Apigenin (C42)	DDX39B
M5		Apigenin (C42)	HGF
M5		Apigenin (C42)	GSTM2
M5		Apigenin (C42)	G6PD
M5		Apigenin (C42)	GSTM1
M5		Apigenin (C42)	PMS2
M5		Apigenin (C42)	TNF
M5		Apigenin (C42)	IL2
M5		Apigenin (C42)	XDH
M6		Genkwani (C21)	SHBG
M6		Genkwani (C21)	GSTM1
M6		Genkwani (C21)	GSTM2
M6		Genkwani (C21)	G6PD
M6		Genkwani (C21)	PMS2
M6		Genkwani (C21)	TNF
M6		Genkwani (C21)	IL2
M6		Genkwani (C21)	PTGS2
M6		Genkwani (C21)	XDH
M9		Apigenin (C42)	CCL5
M9		Apigenin (C42)	HGF
M9		Apigenin (C42)	REN
M9		Apigenin (C42)	DDX39B
M9		Apigenin (C42)	GSTM1
M9		Apigenin (C42)	G6PD
M9		Apigenin (C42)	PMS2
M9		Apigenin (C42)	TNF
M9		Apigenin (C42)	IL2
M9		Apigenin (C42)	XDH
M9		Apigenin (C42)	PTGS2
M10		Apigenin (C42)	AHCY
M10		Apigenin (C42)	SOD2
M10		Apigenin (C42)	PAH
M10		Apigenin (C42)	IGF1
M10		Apigenin (C42)	KIT
M10		Apigenin (C42)	TPH1
M10		Apigenin (C42)	GSTM2
M10		Apigenin (C42)	TNF

M10		Apigenin (C42)	IL2
M10		Apigenin (C42)	XDH
M10		Apigenin (C42)	ACHE
M10		Apigenin (C42)	PTGS2
M11		2',4',7-trihydroxyisoflavan	PTPN1
M11		2',4',7-trihydroxyisoflavan	SHBG
M11		2',4',7-trihydroxyisoflavan	DPP4
M11		2',4',7-trihydroxyisoflavan	HSPA1A
M11		2',4',7-trihydroxyisoflavan	G6PD
M11		2',4',7-trihydroxyisoflavan	TYR
M12		7-hydroxy-2',3',4'-trimethoxyisoflavan	SHBG
M12		7-hydroxy-2',3',4'-trimethoxyisoflavan	PAH
M12		7-hydroxy-2',3',4'-trimethoxyisoflavan	DPP4
M12		7-hydroxy-2',3',4'-trimethoxyisoflavan	GSTM2
M12		7-hydroxy-2',3',4'-trimethoxyisoflavan	ESR1
M12		7-hydroxy-2',3',4'-trimethoxyisoflavan	TYR
M12		7-hydroxy-2',3',4'-trimethoxyisoflavan	PTPN22
M12		7-hydroxy-2',3',4'-trimethoxyisoflavan	CASP3
M12		7-hydroxy-2',3',4'-trimethoxyisoflavan	MAPK1
M13		Apigenin (C42)	ESR1
M13		Apigenin (C42)	SHBG
M13		Apigenin (C42)	CDK2
M13		Apigenin (C42)	DPP4
M13		Apigenin (C42)	FKBP1A
M13		Apigenin (C42)	GSTM2
M13		Apigenin (C42)	GSTM1
M13		Apigenin (C42)	TNF
M13		Apigenin (C42)	IL2
M13		Apigenin (C42)	PTGS2
M13		Apigenin (C42)	XDH
M13		Apigenin (C42)	ACHE
M15		7,3',4'-trihydroxyisoflavanone	PTPN1
M15		7,3',4'-trihydroxyisoflavanone	SHBG
M15		7,3',4'-trihydroxyisoflavanone	CBR1
M15		7,3',4'-trihydroxyisoflavanone	CCL5
M15		7,3',4'-trihydroxyisoflavanone	ABO
M15		7,3',4'-trihydroxyisoflavanone	FKBP1A
M15		7,3',4'-trihydroxyisoflavanone	KIT
M15		7,3',4'-trihydroxyisoflavanone	GSTM1
M15		7,3',4'-trihydroxyisoflavanone	PMS2
M15		7,3',4'-trihydroxyisoflavanone	TNF
M15		7,3',4'-trihydroxyisoflavanone	IL2
M15		7,3',4'-trihydroxyisoflavanone	CASP3
M16		Calycosin	SHBG
M16		Calycosin	MMP1
M16		Calycosin	VDR
M16		Calycosin	GSTM1
M18		7,3',4'-trihydroxyisoflavanone	FKBP1A
M18		7,3',4'-trihydroxyisoflavanone	HSPA1A
M18		7,3',4'-trihydroxyisoflavanone	G6PD
M18		7,3',4'-trihydroxyisoflavanone	TNF
M18		7,3',4'-trihydroxyisoflavanone	IL2
M20		Astraisoflavan-7-O- β -D-glucoside(C22)	CDK2
M20		Astraisoflavan-7-O- β -D-glucoside(C22)	SHBG
M20		Astraisoflavan-7-O- β -D-glucoside(C22)	PAH
M20		Astraisoflavan-7-O- β -D-glucoside(C22)	CASP1
M23		Formononetin (C32)	MIF
M23		Formononetin (C32)	ALB

M23		Formononetin (C32)	GSTM1
M23		Formononetin (C32)	GSTM2
M24		Formononetin (C32)	GSTP1
M24		Formononetin (C32)	F2
M24		Formononetin (C32)	SHBG
M24		Formononetin (C32)	MAPK14
M24		Formononetin (C32)	ABO
M24		Formononetin (C32)	VDR
M24		Formononetin (C32)	ESR1
M24		Formononetin (C32)	MAOA
M24		Formononetin (C32)	ESRRA
M24		Formononetin (C32)	ALOX12
M24		Formononetin (C32)	TYR
M24		Formononetin (C32)	MIF
M24		Formononetin (C32)	XDH
M24		Formononetin (C32)	PFKFB3
M24		Formononetin (C32)	IL2
M24		Formononetin (C32)	CBR1
M24		Formononetin (C32)	ABCB1
M24		Formononetin (C32)	ALOX15
M24		Formononetin (C32)	MAOB
M24		Formononetin (C32)	PON1
M24		Formononetin (C32)	ACHE
M24		Formononetin (C32)	PTPN1
M24		Formononetin (C32)	PPARG
M25		2',4',7-trihydroxyisoflavan	DPP4
M25		2',4',7-trihydroxyisoflavan	HSPA1A
M25		2',4',7-trihydroxyisoflavan	HSPA1B
M25		2',4',7-trihydroxyisoflavan	NOS2
M25		2',4',7-trihydroxyisoflavan	ABO
M25		2',4',7-trihydroxyisoflavan	PNMT
M25		2',4',7-trihydroxyisoflavan	GSTM1
M25		2',4',7-trihydroxyisoflavan	TYR
M25		2',4',7-trihydroxyisoflavan	ESR1
M26		2',4',7-trihydroxyisoflavan	PTPN1
M26		2',4',7-trihydroxyisoflavan	HSPA1A
M26		2',4',7-trihydroxyisoflavan	GSTM1
M26		2',4',7-trihydroxyisoflavan	G6PD
M26		2',4',7-trihydroxyisoflavan	PMS2
M26		2',4',7-trihydroxyisoflavan	TYR
M26		2',4',7-trihydroxyisoflavan	MMP1
M26		2',4',7-trihydroxyisoflavan	CASP3
M27		Methylnissolin	CDK2
M27		Methylnissolin	PTPN1
M27		Methylnissolin	SHBG
M27		Methylnissolin	CCL5
M27		Methylnissolin	ABO
M27		Methylnissolin	RORA
M28		Calycosin	REN
M28		Calycosin	IGF1
M28		Calycosin	CASP1
M28		Calycosin	PMS2
M29		Astraisoflavan	PAH
M29		Astraisoflavan	PIK3R1
M29		Astraisoflavan	GSTM2
M29		Astraisoflavan	GSTM1
M29		Astraisoflavan	TAP1
M29		Astraisoflavan	PMS2

M29		Astraisoflavan	TYR
M29		Astraisoflavan	ESR1
M30		Methylnissolin	CASP7
M30		Methylnissolin	PAH
M30		Methylnissolin	CCL5
M30		Methylnissolin	NOS2
M30		Methylnissolin	ALOX15
M30		Methylnissolin	ALOX12
M30		Methylnissolin	PIK3R1
M30		Methylnissolin	CDK2
M30		Methylnissolin	MIF
M30		Methylnissolin	MAOB
M30		Methylnissolin	MMP1
M30		Methylnissolin	MTOR
M30		Methylnissolin	PIK3CD
M30		Methylnissolin	PIK3CB
M30		Methylnissolin	PIK3CG
M30		Methylnissolin	PIK3CA
M30		Methylnissolin	TYR
M30		Methylnissolin	SYK
M30		Methylnissolin	COMT
M30		Methylnissolin	CASP3
M30		Methylnissolin	BRAF
M30		Methylnissolin	CDK2
M30		Methylnissolin	AKT1
M30		Methylnissolin	MAPK1
M30		Methylnissolin	PDE10A
M31		Formononetin (C32)	ESR1
M31		Formononetin (C32)	HSPA1A
M31		Formononetin (C32)	HSPA1B
M31		Formononetin (C32)	PMS2
M32		Formononetin (C32)	ALB
M32		Formononetin (C32)	MIF
M32		Formononetin (C32)	FKBP1A
M32		Formononetin (C32)	REN
M32		Formononetin (C32)	PNMT
M32		Formononetin (C32)	IL2
M32		Formononetin (C32)	CBR1
M32		Formononetin (C32)	ESRRA
M32		Formononetin (C32)	ALOX12
M32		Formononetin (C32)	MIF
M32		Formononetin (C32)	TYR
M32		Formononetin (C32)	PFKFB3
M32		Formononetin (C32)	MAOA