

Supplementary Table 1.

Mol ID	Molecule Name	Source	191 Targets
MOL000098	quercetin	Astragalus membranaceus	PYGM
MOL000354	isorhamnetin	Astragalus membranaceus	PPARD
MOL000239	Jaranol	Astragalus membranaceus	F7
MOL000371	3,9-di-O-methylnissolin	Astragalus membranaceus	MAOB
MOL000378	7-O-methylisomucronulatol	Astragalus membranaceus	GRIA2
MOL000379	9,10-dimethoxypterocarpan-3-O-β-D-glucoside	Astragalus membranaceus	NCF1
MOL000380	(6aR,11aR)-9,10-dimethoxy-6a,11a-dihydro-6H-benzofurano[3,2-c]chromen-3-ol	Astragalus membranaceus	OLR1
MOL000387	Bifendate	Astragalus membranaceus	ADRB1
MOL000392	formononetin	Astragalus membranaceus	RXRB
MOL000398	isoflavanone	Astragalus membranaceus	KDR
MOL000417	Calycosin	Astragalus membranaceus	PKIA
MOL000422	kaempferol	Astragalus membranaceus	ATP5F1B
MOL000438	(3R)-3-(2-hydroxy-3,4-dimethoxyphenyl)chroman-7-ol	Astragalus membranaceus	HSD3B2
MOL000442	1,7-Dihydroxy-3,9-dimethoxy pterocarpene	Astragalus membranaceus	HSD3B1
MOL001601	1,2,5,6-tetrahydrotanshinone	Salvia miltiorrhiza	IKKB
MOL001942	isoimperatorin	Salvia miltiorrhiza	BAX
MOL002222	sugiol	Salvia miltiorrhiza	MAPK8
MOL002651	Dehydrotanshinone II A	Salvia miltiorrhiza	STAT1
MOL000006	luteolin	Salvia miltiorrhiza	SELE
MOL007036	5,6-dihydroxy-7-isopropyl-1,1-dimethyl-2,3-dihydrophenanthren-4-one	Salvia miltiorrhiza	VCAM1
MOL007041	2-isopropyl-8-methylphenanthrene-3,4-dione	Salvia miltiorrhiza	CYP1B1
MOL007045	3α-hydroxytanshinonella	Salvia miltiorrhiza	HAS2
MOL007048	(E)-3-[2-(3,4-dihydroxyphenyl)-7-hydroxy-benzofuran-4-yl]acrylic acid	Salvia miltiorrhiza	AHR
MOL007049	4-methylenemiltirone	Salvia miltiorrhiza	PSMD3
MOL007050	2-(4-hydroxy-3-methoxyphenyl)-5-(3-hydroxypropyl)-7-methoxy-3-benzofurancarboxaldehyde	Salvia miltiorrhiza	NR1I3
MOL007058	formyltanshinone	Salvia miltiorrhiza	DIO1
MOL007059	3-beta-Hydroxymethylenetanshinquinone	Salvia miltiorrhiza	GSTM1
MOL007061	Methylenetanshinquinone	Salvia miltiorrhiza	GSTM2
MOL007063	przewalskin a	Salvia miltiorrhiza	AKR1C3
MOL007064	przewalskin b	Salvia miltiorrhiza	SLPI
MOL007068	Przewaquinone B	Salvia miltiorrhiza	MMP3
MOL007069	przewaquinone c	Salvia miltiorrhiza	EIF6
MOL007070	(6S,7R)-6,7-dihydroxy-1,6-dimethyl-8,9-dihydro-7H-naphtho[8,7-g]benzofuran-10,11-dione	Salvia miltiorrhiza	PLAU
MOL007071	przewaquinone f	Salvia miltiorrhiza	EGF
MOL007077	sclareol	Salvia miltiorrhiza	ELK1
MOL007079	tanshinaldehyde	Salvia miltiorrhiza	POR
MOL007081	Danshenol B	Salvia miltiorrhiza	ODC1
MOL007082	Danshenol A	Salvia miltiorrhiza	CASP8
MOL007085	Salvilene	Salvia miltiorrhiza	RAF1

Supplementary Table 1. Continued

Mol ID	Molecule Name	Source	191 Targets
MOL007088	cryptotanshinone	Salvia miltiorrhiza	SOD1
MOL007093	dan-shexinkum d	Salvia miltiorrhiza	PRKCA
MOL007094	danshenspiroketallactone	Salvia miltiorrhiza	HIF1A
MOL007098	deoxyneocryptotanshinone	Salvia miltiorrhiza	RUNX1T1
MOL007100	dihydrotanshinlactone	Salvia miltiorrhiza	ACACA
MOL007101	dihydrotanshinone I	Salvia miltiorrhiza	CAV1
MOL007105	epidanshenspiroketallactone	Salvia miltiorrhiza	F3
MOL007108	isocryptotanshinone	Salvia miltiorrhiza	GJA1
MOL007111	Isotanshinone II	Salvia miltiorrhiza	IL1B
MOL007118	microstegiol	Salvia miltiorrhiza	CCL2
MOL007119	miltionone I	Salvia miltiorrhiza	PTGER3
MOL007120	miltionone II	Salvia miltiorrhiza	CXCL8
MOL007121	miltipolone	Salvia miltiorrhiza	PRKCB
MOL007122	Miltirone	Salvia miltiorrhiza	DUOX2
MOL007123	miltirone II	Salvia miltiorrhiza	NOS3
MOL007124	neocryptotanshinone ii	Salvia miltiorrhiza	HSPB1
MOL007125	neocryptotanshinone	Salvia miltiorrhiza	PLAT
MOL007127	1-methyl-8,9-dihydro-7H-naphtho[5,6-g]benzofuran-6,10,11-trione	Salvia miltiorrhiza	THBD
MOL007130	prolithospermic acid	Salvia miltiorrhiza	SERPINE1
MOL007132	(2R)-3-(3,4-dihydroxyphenyl)-2-[(Z)-3-(3,4-dihydroxyphenyl)acryloyl]oxypropionic acid	Salvia miltiorrhiza	COL1A1
MOL007140	(Z)-3-[2-[(E)-2-(3,4-dihydroxyphenyl)vinyl]-3,4-dihydroxy-phenyl]acrylic acid	Salvia miltiorrhiza	IL1A
MOL007141	salvianolic acid g	Salvia miltiorrhiza	MPO
MOL007143	salvilenone I	Salvia miltiorrhiza	NFE2L2
MOL007145	salviolone	Salvia miltiorrhiza	NQO1
MOL007149	NSC 122421	Salvia miltiorrhiza	PARP1
MOL007150	(6S)-6-hydroxy-1-methyl-6-methylol-8,9-dihydro-7H-naphtho[8,7-g]benzofuran-10,11-quinone	Salvia miltiorrhiza	COL3A1
MOL007151	Tanshindiol B	Salvia miltiorrhiza	CXCL11
MOL007152	Przewaquinone E	Salvia miltiorrhiza	CXCL2
MOL007154	tanshinone iia	Salvia miltiorrhiza	DCAF5
MOL007155	(6S)-6-(hydroxymethyl)-1,6-dimethyl-8,9-dihydro-7H-naphtho[8,7-g]benzofuran-10,11-dione	Salvia miltiorrhiza	CHEK2
MOL007156	tanshinone VI	Salvia miltiorrhiza	CLDN4
			PPARA
			HSF1
			CXCL10
			CHUK
			SPP1
			RUNX2
			RASSF1
			E2F1
			E2F2

Supplementary Table 1. Continued

Mol ID	Molecule Name	Source	191 Targets
			ACP3
			CTSD
			IGFBP3
			IGF2
			IRF1
			ERBB3
			PON1
			PCOLCE
			NPEPPS
			HK2
			RASA1
			PTGS1
			CHRM3
			CHRM1
			SCN5A
			CHRM5
			PTGS2
			HTR3A
			CHRM4
			RXRA
			OPRD1
			ADRA1A
			CHRM2
			ADRA1B
			SLC6A3
			ADRB2
			ADRA1D
			OPRM1
			GABRA1
			NCOA2
			NCOA1
			SLC6A4
			ACHE
			ESR1
			AR
			PPARG
			RELA
			EGFR
			AKT1
			VEGFA
			CCND1

Supplementary Table 1. Continued

Mol ID	Molecule Name	Source	191 Targets
			BCL2L1
			CDKN1A
			CASP9
			MMP2
			MMP9
			MAPK1
			IL10
			RB1
			TNF
			IL6
			CASP3
			TP53
			NFKBIA
			TOP1
			MMP1
			ERBB2
			HMOX1
			ICAM1
			BIRC5
			IL2
			CCNB1
			IFNG
			IL4
			TOP2A
			GSTP1
			SLC2A4
			INSR
			CD40LG
			MET
			CCNA2
			ADRA2C
			NOS2
			ESR2
			MAPK14
			GSK3B
			PGR
			KCNH2
			CHEK1
			SLC6A2
			BCL2
			AHSA1

Supplementary Table 1. Continued

Mol ID	Molecule Name	Source	191 Targets
			CYP3A4
			CYP1A2
			MYC
			CYP1A1
			NR1I2
			DRD2
			MDM2
			PCNA
			CASP7
			MCL1
			TYR
			PTGES
			NUF2
			ADCY2
			ADRA2A
			NR3C2
			NR3C1
			STAT3
			EDN1
			CHRNA2
			DRD5
			ADRA2B
			GABRG3
			GABRE
			FASN
			EDNRA
			NPM1
			ECE1
			CALCR
			ITGB3

Supplementary Table 2.

158 intersection targets
PYGM
PPARD
F7
MAOB
NCF1
OLR1
ADRB1
KDR
HSD3B2
HSD3B1
IKBKB
BAX
MAPK8
STAT1
SELE
VCAM1
CYP1B1
AHR
NR1I3
GSTM1
SLPI
MMP3
PLAU
EGF
POR
ODC1
CASP8
RAF1
SOD1
PRKCA
HIF1A
RUNX1T1
CAV1
F3
GJA1
IL1B
CCL2
PTGER3
CXCL8
PRKCB
DUOX2

Supplementary Table 2. Continued

158 intersection targets
NOS3
HSPB1
PLAT
THBD
SERPINE1
COL1A1
IL1A
MPO
NFE2L2
NQO1
PARP1
COL3A1
CXCL2
CHEK2
PPARA
HSF1
CXCL10
CHUK
SPP1
RUNX2
RASSF1
E2F1
CTSD
IGFBP3
IGF2
IRF1
ERBB3
PON1
HK2
RASA1
PTGS1
CHRM3
CHRM1
SCN5A
PTGS2
HTR3A
RXRA
OPRD1
ADRA1A
CHRM2
SLC6A3

Supplementary Table 2. Continued

158 intersection targets
ADRB2
OPRM1
SLC6A4
ACHE
ESR1
AR
PPARG
RELA
EGFR
AKT1
VEGFA
CCND1
BCL2L1
CDKN1A
CASP9
MMP2
MMP9
MAPK1
IL10
RB1
TNF
IL6
CASP3
TP53
NFKBIA
TOP1
MMP1
ERBB2
HMOX1
ICAM1
BIRC5
IL2
CCNB1
IFNG
IL4
TOP2A
GSTP1
SLC2A4

Supplementary Table 2. Continued

158 intersection targets
INSR
CD40LG
MET
CCNA2
ADRA2C
NOS2
ESR2
MAPK14
GSK3B
PGR
KCNH2
CHEK1
SLC6A2
BCL2
CYP3A4
CYP1A2
MYC
CYP1A1
NR1I2
DRD2
MDM2
PCNA
CASP7
MCL1
TYR
ADRA2A
NR3C2
NR3C1
STAT3
EDN1
DRD5
ADRA2B
FASN
EDNRA
NPM1
ECE1
CALCR
ITGB3