

Exploration of the Potential Targets and Molecular Mechanism of *Carthamus tinctorius* L. for Liver Fibrosis Based on Network Pharmacology and Molecular Docking Strategy

Table S1. The bioactive components and treating targets of HH.

components	Tar-gets	Uni-prot ID	components	Targets	Uniprot ID
poriferast-5-en-3beta-ol	HMG CR	P04035	phytofluene	ACACB	O00763
poriferast-5-en-3beta-ol	CYP51A1	Q16850	phytofluene	FAAH	O00519
poriferast-5-en-3beta-ol	AR	P10275	phytofluene	KDR	P35968
poriferast-5-en-3beta-ol	NPC1L1	Q9UHC9	phytofluene	FGFR1	P11362
poriferast-5-en-3beta-ol	NR1H3	Q13133	phytofluene	PLA2G2A	P14555
poriferast-5-en-3beta-ol	CYP17A1	P05093	phytofluene	PTGS2	P35354
poriferast-5-en-3beta-ol	RORC	P51449	phytofluene	TRPV1	Q8NER1
poriferast-5-en-3beta-ol	CYP19A1	P11511	Pyrethrin II	GRM5	P41594
poriferast-5-en-3beta-ol	ESR2	Q92731	Pyrethrin II	HCRTR2	O43614
poriferast-5-en-3beta-ol	ESR1	P03372	Pyrethrin II	HCRTR1	O43613
poriferast-5-en-3beta-ol	SHBG	P04278	Pyrethrin II	CAPN1	P07384
poriferast-5-en-3beta-ol	SREBF2	Q12772	Pyrethrin II	MAPK8	P45983
poriferast-5-en-3beta-ol	CYP2C19	P33261	Pyrethrin II	MAPK10	P53779
poriferast-5-en-3beta-ol	SLC6A2	P23975	Pyrethrin II	SCN9A	Q15858
poriferast-5-en-3beta-ol	BCHE	P06276	Pyrethrin II	PTGER1	P34995
Flavoxanthin	VDR	P11473	Pyrethrin II	CFD	P00746
Flavoxanthin	ALOX5	P09917	Pyrethrin II	CAPN1 CAPNS1	P07384 P04632
Flavoxanthin	PRKCG	P05129	Pyrethrin II	CTSL	P07711
Flavoxanthin	PRKCB	P05771	Pyrethrin II	CTSS	P25774
Flavoxanthin	CHEK1	O14757	Pyrethrin II	PARP1	P09874
Flavoxanthin	GLS	O94925	Pyrethrin II	CTSB	P07858
Flavoxanthin	ACHE	P22303	Pyrethrin II	PPARG	P37231

Flavoxanthin	BCL2	P10415	6-Hydroxykaempferol	AKR1B1	P15121
Flavoxanthin	SF3B3	Q15393	6-Hydroxykaempferol	NOX4	Q9NPH5
Flavoxanthin	CHRM5	P08912	6-Hydroxykaempferol	XDH	P47989
Flavoxanthin	CHRM2	P08172	6-Hydroxykaempferol	FLT3	P36888
Flavoxanthin	ENPP2	Q13822	6-Hydroxykaempferol	CA2	P00918
Flavoxanthin	CHRM4	P08173	6-Hydroxykaempferol	ALOX5	P09917
Flavoxanthin	CHRM1	P11229	6-Hydroxykaempferol	CA7	P43166
Flavoxanthin	CHRM3	P20309	6-Hydroxykaempferol	HSD17B2	P37059
4-[(E)-4-(3,5-dimethoxy-4-oxo-1-cyclohexa-2,5-dienylidene)but-2-enylidene]-2,6-dimethoxycyclohexa-2,5-dien-1-one	CHRM2	P08172	6-Hydroxykaempferol	ABCC1	P33527
4-[(E)-4-(3,5-dimethoxy-4-oxo-1-cyclohexa-2,5-dienylidene)but-2-enylidene]-2,6-dimethoxycyclohexa-2,5-dien-1-one	CHRM1	P11229	6-Hydroxykaempferol	CA12	O43570
4-[(E)-4-(3,5-dimethoxy-4-oxo-1-cyclohexa-2,5-dienylidene)but-2-enylidene]-2,6-dimethoxycyclohexa-2,5-dien-1-one	TAAR1	Q96RJ0	6-Hydroxykaempferol	ABCB1	P08183
4-[(E)-4-(3,5-dimethoxy-4-oxo-1-cyclohexa-2,5-dienylidene)but-2-enylidene]-2,6-dimethoxycyclohexa-2,5-dien-1-one	PDE10A	Q9Y233	6-Hydroxykaempferol	CYP1B1	Q16678
4-[(E)-4-(3,5-dimethoxy-4-oxo-1-cyclohexa-2,5-dienylidene)but-2-enylidene]-2,6-dimethoxycyclohexa-2,5-dien-1-one	FAP	Q12884	6-Hydroxykaempferol	ABCG2	Q9UNQ0
4-[(E)-4-(3,5-dimethoxy-4-oxo-1-cyclohexa-2,5-dienylidene)but-2-enylidene]-2,6-dimethoxycyclohexa-2,5-dien-1-one	EZR	P15311	6-Hydroxykaempferol	PFKFB3	Q16875
4-[(E)-4-(3,5-dimethoxy-4-oxo-1-cyclohexa-2,5-dienylidene)but-2-enylidene]-2,6-dimethoxycyclohexa-2,5-dien-1-one	ABCB1	P08183	6-Hydroxykaempferol	ADORA1	P30542
4-[(E)-4-(3,5-dimethoxy-4-oxo-1-cyclohexa-2,5-dienylidene)but-2-enylidene]-2,6-dimethoxycyclohexa-2,5-dien-1-one	PTGS2	P35354	baicalein	KDM4E	B2RXH2
4-[(E)-4-(3,5-dimethoxy-4-oxo-1-cyclohexa-2,5-dienylidene)but-2-enylidene]-2,6-dimethoxycyclohexa-2,5-dien-1-one	ABCC1	P33527	baicalein	XDH	P47989
4-[(E)-4-(3,5-dimethoxy-4-oxo-1-cyclohexa-2,5-dienylidene)but-2-enylidene]-2,6-dimethoxycyclohexa-2,5-dien-1-one	PREP	P48147	baicalein	ALOX15	P16050
4-[(E)-4-(3,5-dimethoxy-4-oxo-1-cyclohexa-2,5-dienylidene)but-2-enylidene]-2,6-dimethoxycyclohexa-2,5-dien-1-one	MET	P08581	baicalein	CDK1	P06493
4-[(E)-4-(3,5-dimethoxy-4-oxo-1-cyclohexa-2,5-dienylidene)but-2-enylidene]-2,6-dimethoxycyclohexa-2,5-dien-1-one	SCN9A	Q15858	baicalein	ALOX12	P18054
4-[(E)-4-(3,5-dimethoxy-4-oxo-1-cyclohexa-2,5-dienylidene)but-2-enylidene]-2,6-dimethoxycyclohexa-2,5-dien-1-one	FKBP1A	P62942	baicalein	GRK6	P43250
4-[(E)-4-(3,5-dimethoxy-4-oxo-1-cyclohexa-2,5-dienylidene)but-2-enylidene]-2,6-dimethoxycyclohexa-2,5-dien-1-one	HTR2A	P28223	baicalein	CYP19A1	P11511

4-[(E)-4-(3,5-dimethoxy-4-oxo-1-cyclohexa-2,5-dienylidene)but-2-enylidene]-2,6-dimethoxycyclohexa-2,5-dien-1-one	PIM1	P11309	baicalein	CA7	P43166
lignan	NR3C1	P04150	baicalein	CA12	O43570
lignan	PDE5A	O76074	baicalein	CA4	P22748
lignan	SYK	P43405	baicalein	ABCB1	P08183
lignan	CYP2C9	P11712	baicalein	CYP1B1	Q16678
lignan	CYP2C19	P33261	baicalein	HSD17B1	P14061
lignan	TRPV1	Q8NER1	baicalein	AKR1B1	P15121
lignan	MTO	P42345	baicalein	CDK5R1 CDK5	Q15078 Q00535
lignan	PIK3CA	P42336	qt_carthamone	IGFBP3	P17936
lignan	RORC	P51449	qt_carthamone	AKR1C3	P42330
lignan	PDE7A	Q13946	qt_carthamone	NOX4	Q9NPH5
lignan	CYP3A4	P08684	qt_carthamone	CAMKK2	Q96RR4
lignan	CHRM2	P08172	qt_carthamone	LCK	P06239
lignan	BRD2	P25440	qt_carthamone	SELL	P14151
lignan	CFD	P00746	qt_carthamone	SELE	P16581
lignan	CDK2	P24941	qt_carthamone	SELP	P16109
lupeol-palmitate	HSD11B1	P28845	qt_carthamone	MMP16	P51512
lupeol-palmitate	F2	P00734	qt_carthamone	MMP13	P45452
lupeol-palmitate	PRSS1	P07477	qt_carthamone	MMP1	P03956
lupeol-palmitate	CTRC	Q99895	qt_carthamone	MMP2	P08253
lupeol-palmitate	PTPN1	P18031	qt_carthamone	MMP14	P50281
lupeol-palmitate	VDR	P11473	qt_carthamone	MMP8	P22894
lupeol-palmitate	PREP	P48147	qt_carthamone	AKR1B1	P15121
lupeol-palmitate	CDC25A	P30304	6-Hydroxynaringenin	CYP19A1	P11511
lupeol-palmitate	PTGES	O14684	6-Hydroxynaringenin	CA7	P43166
lupeol-palmitate	TOP2A	P11388	6-Hydroxynaringenin	CA12	O43570
lupeol-palmitate	PTGS2	P35354	6-Hydroxynaringenin	CA4	P22748
lupeol-palmitate	AR	P10275	6-Hydroxynaringenin	CYP1B1	Q16678

lupeol-palmitate	CYP17A1	P05093	6-Hydroxynaringenin	ESR1	P03372
lupeol-palmitate	HMGCR	P04035	6-Hydroxynaringenin	MAOB	P27338
lupeol-palmitate	CYP19A1	P11511	6-Hydroxynaringenin	PTGS1	P23219
Phytoene	ADORA1	P30542	6-Hydroxynaringenin	HSD17B1	P14061
Phytoene	ADORA2A	P29274	6-Hydroxynaringenin	TAS2R31	P59538
Phytoene	ADORA3	P0DMS8	6-Hydroxynaringenin	ESR2	Q92731
Phytoene	SPHK2	Q9NRA0	6-Hydroxynaringenin	ABCC1	P33527
Phytoene	RBP4	P02753	6-Hydroxynaringenin	SHBG	P04278
Phytoene	PPARA	Q07869	6-Hydroxynaringenin	CBR1	P16152
Phytoene	DNM1	Q05193	6-Hydroxynaringenin	ABCG2	Q9UNQ0
Phytoene	MOGAT2	Q3SYC2	quercetagenin	PIM1	P11309
Phytoene	ENPP2	Q13822	quercetagenin	AKR1B1	P15121
Phytoene	TACR3	P29371	quercetagenin	MAPT	P10636
Phytoene	BDKRB2	P30411	quercetagenin	KDM4E	B2RXH2
Phytoene	HDAC1	Q13547	quercetagenin	GPR35	Q9HC97
Phytoene	HDAC4	P56524	quercetagenin	TOP2A	P11388
Phytoene	NPY5R	Q15761	quercetagenin	XDH	P47989
Phytoene	TOP2A	P11388	quercetagenin	FLT3	P36888
phytofluene	ADORA1	P30542	quercetagenin	INSR	P06213
phytofluene	ADORA2A	P29274	quercetagenin	ACHE	P22303
phytofluene	ADORA3	P0DMS8	quercetagenin	GLO1	Q04760
phytofluene	SPHK2	Q9NRA0	quercetagenin	MYLK	Q15746
phytofluene	RBP4	P02753	quercetagenin	SYK	P43405
phytofluene	DNM1	Q05193	quercetagenin	ABCC1	P33527
phytofluene	CNR1	P21554	quercetagenin	PIK3CG	P48736
phytofluene	ENPP2	Q13822	7,8-dimethyl-1H-pyrimido[5,6-g]quinoxaline-2,4-dione	CHEK1	O14757
7,8-dimethyl-1H-pyrimido[5,6-g]quinoxaline-2,4-dione	PARP14	Q460N5	7,8-dimethyl-1H-pyrimido[5,6-g]quinoxaline-2,4-dione	CYP11B2	P19099
7,8-dimethyl-1H-pyrimido[5,6-g]quinoxaline-2,4-	PARP	Q460	7,8-dimethyl-1H-	HSP90AA1	P07900

dione	15	N3	pyrimido[5,6-g]quinoxaline-2,4-dione		
7,8-dimethyl-1H-pyrimido[5,6-g]quinoxaline-2,4-dione	PARP10	Q53GL7	7,8-dimethyl-1H-pyrimido[5,6-g]quinoxaline-2,4-dione	FBP1	P09467
7,8-dimethyl-1H-pyrimido[5,6-g]quinoxaline-2,4-dione	CCND1 CDK4	P24385 P11802	luteolin	NOX4	Q9NPH5
7,8-dimethyl-1H-pyrimido[5,6-g]quinoxaline-2,4-dione	HTR2C	P28335	luteolin	AKR1B1	P15121
7,8-dimethyl-1H-pyrimido[5,6-g]quinoxaline-2,4-dione	PARP1	P09874	luteolin	CDK5R1 CDK5	Q15078 Q00535
7,8-dimethyl-1H-pyrimido[5,6-g]quinoxaline-2,4-dione	GSK3B	P49841	luteolin	XDH	P47989
7,8-dimethyl-1H-pyrimido[5,6-g]quinoxaline-2,4-dione	SIRT2	Q8IXJ6	luteolin	MAOA	P21397
7,8-dimethyl-1H-pyrimido[5,6-g]quinoxaline-2,4-dione	ASAHI	Q13510	luteolin	FLT3	P36888
7,8-dimethyl-1H-pyrimido[5,6-g]quinoxaline-2,4-dione	CISD1	Q9NZ45	luteolin	CA2	P00918
7,8-dimethyl-1H-pyrimido[5,6-g]quinoxaline-2,4-dione	PIK3CD	O00329	luteolin	CCNB3 CDK1 CCNB1 CCNB2	Q8WWL7 P06493 P14635 O95067
beta-carotene	RBP4	P02753	luteolin	ALOX5	P09917
beta-carotene	ADORA1	P30542	luteolin	ADORA1	P30542
beta-carotene	ADORA2A	P29274	luteolin	CA7	P43166
beta-carotene	ADORA3	P0DMS8	luteolin	GLO1	Q04760
beta-carotene	AR	P10275	luteolin	APP	P05067
beta-carotene	CYP19A1	P11511	luteolin	SYK	P43405
beta-carotene	ESR1	P03372	luteolin	GSK3B	P49841
beta-carotene	ESR2	Q92731	CLR	CYP51A1	Q16850
beta-carotene	RORC	P51449	CLR	HMGCR	P04035
beta-carotene	HTR2B	P41595	CLR	CYP17A1	P05093
beta-carotene	RXRB	P28702	CLR	AR	P10275
beta-carotene	ADRA2B	P18089	CLR	ESR2	Q92731
beta-carotene	RARG	P13631	CLR	ESR1	P03372
beta-carotene	RXRG	P48443	CLR	SHBG	P04278
beta-carotene	RARB	P10826	CLR	NR1H3	Q13133
Baicalin	AKR1B1	P15121	CLR	NPC1L1	Q9UHC9

Baicalin	ADO RA1	P3054 2	CLR	SREBF2	Q12772
Baicalin	TNF	P0137 5	CLR	CYP19A1	P11511
Baicalin	IL2	P6056 8	CLR	RORC	P51449
Baicalin	XDH	P4798 9	CLR	SLC6A4	P31645
Baicalin	PTGS 2	P3535 4	CLR	SLC6A2	P23975
Baicalin	RPS6 KA3	P5181 2	CLR	CHRM2	P08172
Baicalin	EGFR	P0053 3	quercetin	NOX4	Q9NPH5
Baicalin	ACH E	P2230 3	quercetin	AVPR2	P30518
Baicalin	NQO 2	P1608 3	quercetin	AKR1B1	P15121
Baicalin	NMU R2	Q9GZ Q4	quercetin	XDH	P47989
Baicalin	ADR A2A	P0891 3	quercetin	MAOA	P21397
Baicalin	ADR A2C	P1882 5	quercetin	IGF1R	P08069
Baicalin	NOX4	Q9NP H5	quercetin	FLT3	P36888
Baicalin	ALD H2	P0509 1	quercetin	CYP19A1	P11511
beta-sitosterol	HMG CR	P0403 5	quercetin	EGFR	P00533
beta-sitosterol	CYP5 1A1	Q1685 0	quercetin	F2	P00734
beta-sitosterol	AR	P1027 5	quercetin	CA2	P00918
beta-sitosterol	NPC1 L1	Q9U HC9	quercetin	PIM1	P11309
beta-sitosterol	NR1H 3	Q1313 3	quercetin	ALOX5	P09917
beta-sitosterol	CYP1 7A1	P0509 3	quercetin	AURKB	Q96GD4
beta-sitosterol	RORC	P5144 9	quercetin	DRD4	P21917
beta-sitosterol	CYP1 9A1	P1151 1	Hydroxysafflor Yellow A	YARS	P54577
beta-sitosterol	ESR2	Q9273 1	Hydroxysafflor Yellow A	MAG	P20916
beta-sitosterol	ESR1	P0337 2	Hydroxysafflor Yellow A	CD22	P20273
beta-sitosterol	SHBG	P0427 8	Hydroxysafflor Yellow A	CA2	P00918
beta-sitosterol	SREB F2	Q1277 2	Hydroxysafflor Yellow A	CA7	P43166
beta-sitosterol	CYP2 C19	P3326 1	Hydroxysafflor Yellow A	CA1	P00915
beta-sitosterol	SLC6 A2	P2397 5	Hydroxysafflor Yellow A	CA3	P07451
beta-sitosterol	BCHE	P0627	Hydroxysafflor Yellow	CA12	O43570

		6	A		
kaempferol	NOX4	Q9NP H5	Hydroxysafflor Yellow A	CA14	Q9ULX7
kaempferol	AKR1 B1	P1512 1	Hydroxysafflor Yellow A	CA9	Q16790
kaempferol	XDH	P4798 9	Hydroxysafflor Yellow A	CA4	P22748
kaempferol	TYR	P1467 9	Hydroxysafflor Yellow A	CA13	Q8N1Q1
kaempferol	FLT3	P3688 8	Hydroxysafflor Yellow A	CA5A	P35218
kaempferol	CA2	P0091 8	Hydroxysafflor Yellow A	PRKCD	Q05655
kaempferol	ALO X5	P0991 7	Hydroxysafflor Yellow A	PTPN1	P18031
kaempferol	CA7	P4316 6	Stigmasterol	CYP51A1	Q16850
kaempferol	HSD1 7B2	P3705 9	Stigmasterol	HMGCR	P04035
kaempferol	ABCC 1	P3352 7	Stigmasterol	NR1H3	Q13133
kaempferol	HSD1 7B1	P1406 1	Stigmasterol	NPC1L1	Q9UHC9
kaempferol	AHR	P3586 9	Stigmasterol	CYP17A1	P05093
kaempferol	CA12	O4357 0	Stigmasterol	AR	P10275
kaempferol	ESRR A	P1147 4	Stigmasterol	SREBF2	Q12772
kaempferol	ABCB 1	P0818 3	Stigmasterol	CYP19A1	P11511
			Stigmasterol	RORC	P51449
			Stigmasterol	ESR1	P03372
			Stigmasterol	ESR2	Q92731
			Stigmasterol	SHBG	P04278
			Stigmasterol	SLC6A2	P23975
			Stigmasterol	SERPINA6	P08185
			Stigmasterol	PTPN1	P18031

Table S2. The disease targets of liver fibrosis.

Targets	Targets	Targets
HMGCR	HSD11B1	SELL
CYP51A1	F2	SELE
AR	PRSS1	SELP
NPC1L1	CTRC	MMP13
NR1H3	PTPN1	MMP1
CYP17A1	CDC25A	MMP2
RORC	TOP2A	MMP14
CYP19A1	ADORA1	MMP8
ESR2	ADORA2A	MAOB
ESR1	SPHK2	PTGS1
SHBG	RBP4	CBR1
SREBF2	PPARA	MAPT
CYP2C19	DNM1	GPR35
BCHE	HDAC1	INSR
VDR	HDAC4	GLO1
ALOX5	CNR1	MYLK
PRKCB	FAAH	PIK3CG
GLS	KDR	CYP11B2
ACHE	FGFR1	HSP90AA1
BCL2	PLA2G2A	GSK3B
ENPP2	CAPN1	SIRT2
CHRM3	MAPK8	ASAH1
FAP	MAPK10	CISD1
EZR	CTSL	HTR2B
ABCB1	PARP1	RXRΒ
PTGS2	CTSB	RARB
ABCC1	PPARG	TNF
PREP	AKR1B1	IL2
MET	NOX4	RPS6KA3
HTR2A	XDH	EGFR
NR3C1	FLT3	ALDH2
PDE5A	CA2	TYR
SYK	CA12	AHR
CYP2C9	CYP1B1	SERPINA6
TRPV1	ABCG2	APP
MTOR	PFKFB3	SLC6A4
PIK3CA	CDK1	AVPR2
CYP3A4	CA4	IGF1R
BRD2	IGFBP3	AURKB
CDK2	CAMKK2	
PRKCD	CA9	