

Supplementary figures

Figure S1

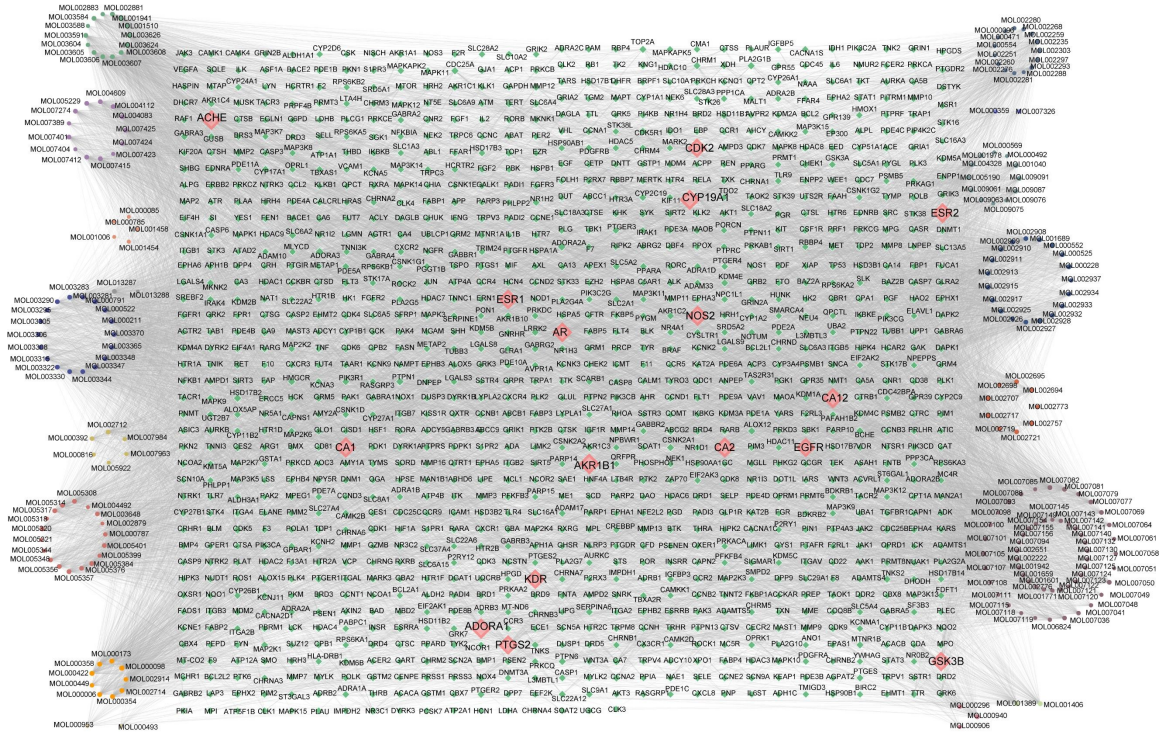


Figure S1. Compound-target network. Circles represent candidate compounds. Diamonds represent candidate targets, pink diamonds represent the top 15 target proteins according to degree, and diamonds with a red border represent the top 15 target proteins according to betweenness centrality. The size of the node is proportional to the value of degree.

Figure S2.

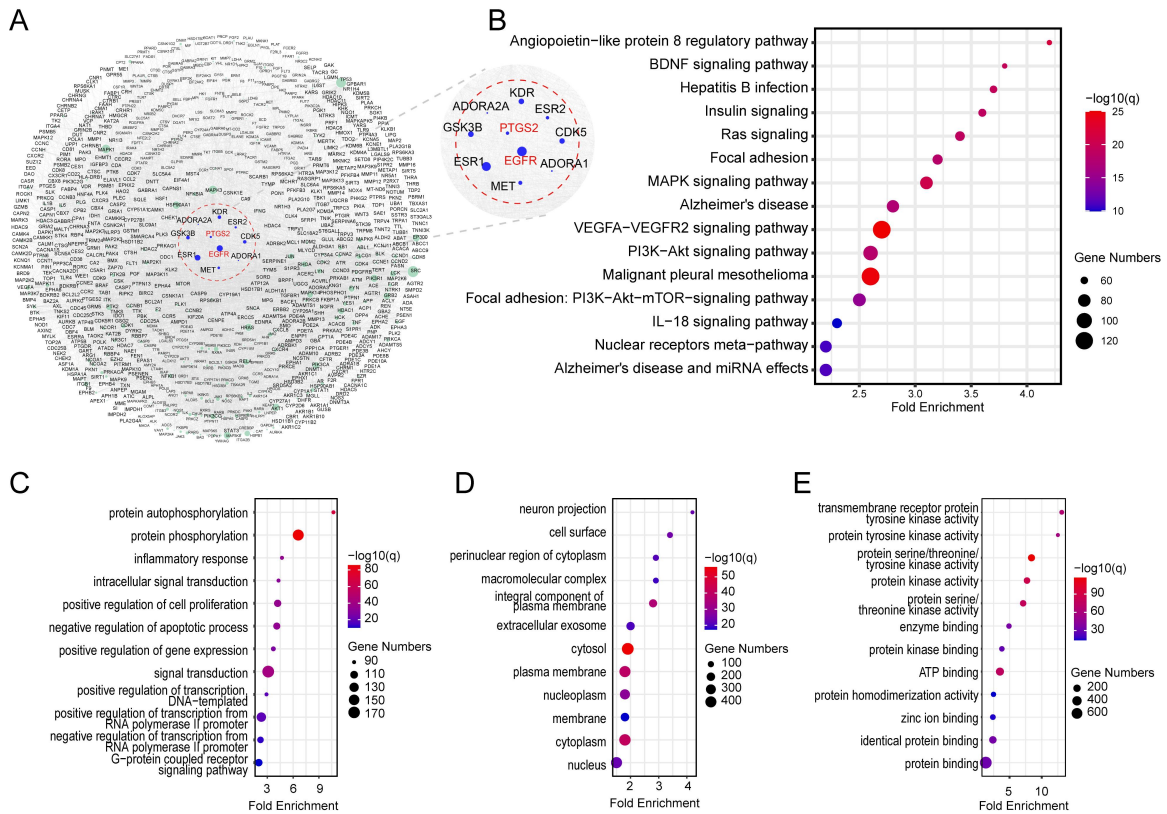


Figure S2. Functional analysis of the compound targets. (A) PPI network of candidate targets. Blue circles represent the hub gene, calculated by Cytohubba. (B) Wiki pathway of top 15 enriched pathways. (C) Top 12 biological processes of G.O. enrichment analysis. (D) Top 12 molecular functions of G.O. enrichment analysis. (E) Top 12 cellular components of G.O. enrichment analysis. Fold enrichment and P-value reflect the degree of importance.

Figure S3.

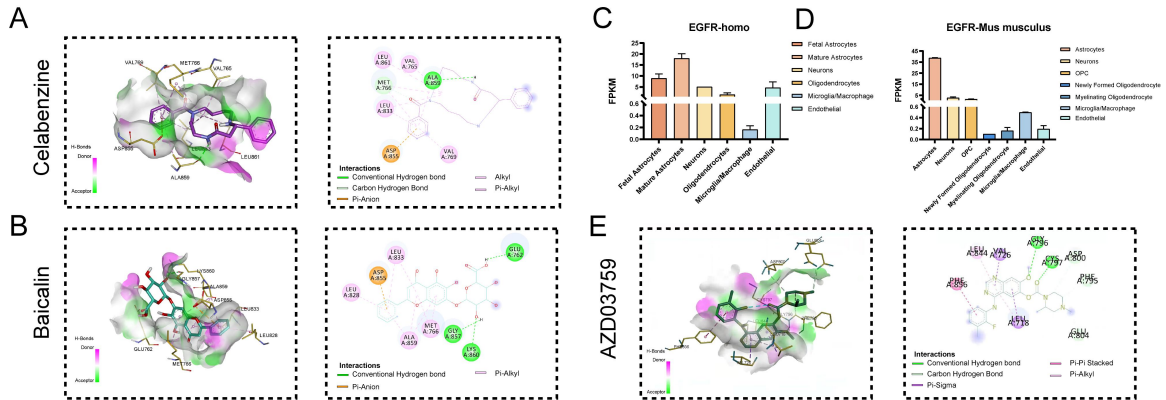


Figure S3. Molecular docking of celabenzine and baicalin with EGFR.

(A) The 3D and 2D interaction diagrams of celabenzine toward EGFR. (B) The 3D and 2D interaction diagrams of baicalin toward EGFR. (C) Brain RNA sequencing results of Homo sapiens. (D) Brain RNA sequencing results of mice; (E) The 3D and 2D interaction diagrams of AZD3759 toward EGFR.

Figure S4.

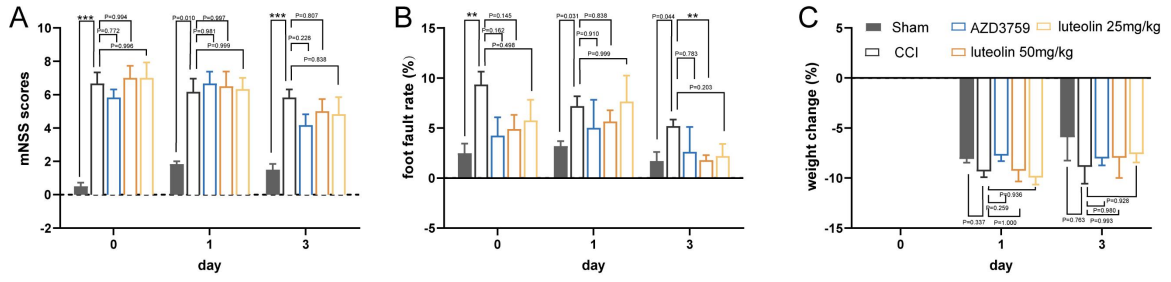


Figure S4. Behavioral tests on days 0, 1, and 3 after CCI. (A)

Neurobehavioral scores, **(B)** foot fault rate, and **(C)** body weight changes.

Data are expressed as the Mean \pm SEM, N = 6, ** $P < 0.01$, *** $P < 0.001$.

Supplementary tables

Table S1. The information about the candidate compound.

Medicinal Plant	Mol ID	Molecule Name	OB (%)	DL	
A. Annuua	MOL000006	luteolin	36.16	0.25	
	MOL000098	quercetin	46.43	0.28	
	MOL000354	isorhamnetin	49.60	0.31	
	MOL000359	sitosterol	36.91	0.75	
	MOL000422	kaempferol	41.88	0.24	
	MOL000449	Stigmasterol	43.83	0.76	
	MOL002235	EUPATIN	50.80	0.41	
	MOL004083	Tamarixetin	32.86	0.31	
	MOL004112	Patuletin	53.11	0.34	
	MOL004609	Areapillin	48.96	0.41	
	MOL005229	Artemetin	49.55	0.48	
	MOL007274	Skrofulein	30.35	0.30	
	MOL007389	artemisitenone	54.36	0.31	
	MOL007400	vicenin-2 Qt	45.84	0.21	
	MOL007401	Cirsiliol	43.46	0.34	
	MOL007404	vitexin Qt	52.18	0.21	
	MOL007412	DMQT	42.60	0.37	
	MOL007415	Asperglauclide	58.02	0.52	
	MOL007423	6,8-di-c-glucosylapigenin Qt	59.85	0.21	
	MOL007424	artemisinin	49.88	0.31	
	MOL007425	dihydroartemisinin	50.75	0.30	
	MOL007426	deoxyartemisinin	54.47	0.26	
	A. Bidentatae	MOL000085	beta-daucosterol Qt	36.91	0.75
		MOL000098	quercetin	46.43	0.28
		MOL000173	wogonin	30.68	0.23
		MOL000358	beta-sitosterol	36.91	0.75
MOL000422		kaempferol	41.88	0.24	
MOL000449		Stigmasterol	43.83	0.76	
MOL000785		palmitate	64.60	0.65	
MOL001006		poriferasta-7,22E-dien-3beta-ol	42.98	0.76	
MOL001454		berberine	36.86	0.78	
MOL001458		coptisine	30.67	0.86	
MOL002643		delta 7-stigmastanol	37.42	0.75	
MOL002714		baicalein	33.52	0.21	
MOL002776		Baicalin	40.12	0.75	

	MOL002897	epiberberine	43.09	0.78
	MOL003847	Inophyllum E	38.81	0.85
	MOL004355	Spinasterol	42.98	0.76
	MOL012461	28-norolean-17-en-3-ol	35.93	0.78
	MOL012505	bidentatoside,ii_qt	31.76	0.59
	MOL012537	Spinoside A	41.75	0.40
	MOL012542	β -ecdysterone	44.23	0.82
C. Asiatica	MOL000098	quercetin	46.43	0.28
	MOL000359	sitosterol	36.91	0.75
	MOL007326	Cynarin(e)	31.76	0.68
C. Longa	MOL000449	Stigmasterol	43.83	0.76
	MOL000493	campesterol	37.58	0.71
	MOL000953	CLR	37.87	0.68
C. Monnieri	MOL000358	beta-sitosterol	36.91	0.75
	MOL000449	Stigmasterol	43.83	0.76
	MOL001510	24-epicampesterol	37.58	0.71
	MOL001771	poriferast-5-en-3beta-ol	36.91	0.75
	MOL001941	Ammidin	34.55	0.22
	MOL002881	Diosmetin	31.14	0.27
	MOL002883	Ethyl oleate (NF)	32.40	0.19
	MOL003584	Xanthoxylin N	35.51	0.21
	MOL003588	Prangenidin	36.31	0.22
	MOL003591	ar-curcumene	52.34	0.65
	MOL003600	cnidimol B	68.66	0.26
	MOL003604	cnidimol F	54.43	0.28
	MOL003605	(E)-2,3-bis(2-keto-7-methoxy-chromen-8-yl)acrolein	56.38	0.71
	MOL003606	cniforin A	55.89	0.47
	MOL003607	cniforin B	36.70	0.60
	MOL003608	O-Acetylcolumbianetin	60.04	0.26
	MOL003617	isogosferol	30.07	0.25
	MOL003624	o-Isovalerylcolum bianetin	64.03	0.36
	MOL003626	Ostruthin	30.65	0.23
C. Sativus	MOL000098	quercetin	46.43	0.28
	MOL000354	isorhamnetin	49.60	0.31
	MOL000422	kaempferol	41.88	0.24
	MOL001389	n-heptanal	79.74	0.59
	MOL001406	crocetin	35.30	0.26
C. Tinctorius	MOL000006	luteolin	36.16	0.25
	MOL000098	quercetin	46.43	0.28
	MOL000358	beta-sitosterol	36.91	0.75

	MOL000422	kaempferol	41.88	0.24
	MOL000449	Stigmasterol	43.83	0.76
	MOL000953	CLR	37.87	0.68
	MOL001771	poriferast-5-en-3beta-ol	36.91	0.75
	MOL002680	Flavoxanthin	60.41	0.56
	MOL002694	4-[(E)-4-(3,5-dimethoxy-4-oxo-1-cyclohexa-2,5-dienylidene)but-2-enylidene]-2,6-dimethoxycyclohexa-2,5-dien-1-one	48.47	0.36
	MOL002695	lignan	43.32	0.65
	MOL002698	lupeol-palmitate	33.98	0.32
	MOL002706	Phytoene	39.56	0.50
	MOL002707	phytofluene	43.18	0.50
	MOL002710	Pyrethrin II	48.36	0.35
	MOL002712	6-Hydroxykaempferol	62.13	0.27
	MOL002714	baicalein	33.52	0.21
	MOL002717	qt_carthamone	51.03	0.20
	MOL002719	6-Hydroxynaringenin	33.23	0.24
	MOL002721	quercetagetin	45.01	0.31
	MOL002757	7,8-dimethyl-1H-pyrimido[5,6-g]quinoxaline-2,4-dione	45.75	0.19
	MOL002773	beta-carotene	37.18	0.58
	MOL002776	Baicalin	40.12	0.75
C. Zedoaria	MOL000296	hederagenin	36.91	0.75
	MOL000906	wenjine	47.93	0.27
	MOL000940	bisdemethoxycurcumin	77.38	0.26
D. Fortune	MOL000006	luteolin	36.16	0.25
	MOL000358	beta-sitosterol	36.91	0.75
	MOL000422	kaempferol	41.88	0.24
	MOL000449	Stigmasterol	43.83	0.76
	MOL000492	(+)-catechin	54.83	0.24
	MOL000569	digallate	61.85	0.26
	MOL001040	(2R)-5,7-dihydroxy-2-(4-hydroxyphenyl)chroman-4-one	42.36	0.21
	MOL001978	Aureusidin	53.42	0.24
	MOL002914	Eriodyctiol (flavanone)	41.35	0.24
	MOL004328	naringenin	59.29	0.21
	MOL005190	eriodictyol	71.79	0.24
	MOL009061	22-Stigmasten-3-one	39.25	0.76
	MOL009063	Cyclolaudenol acetate	41.66	0.79
	MOL009075	cycloartenone	40.57	0.79

	MOL009076	cyclolaudenol	39.05	0.79
	MOL009078	davallioside A Qt	62.65	0.51
	MOL009087	marioside Qt	70.79	0.19
	MOL009091	xanthogalenol	41.08	0.32
E. Breviscapus	MOL000006	luteolin	36.16	0.25
	MOL000098	quercetin	46.43	0.28
	MOL000392	formononetin	69.67	0.21
	MOL000422	kaempferol	41.88	0.24
	MOL000816	ergosta-7,22-dien-3-one	44.88	0.72
	MOL001040	(2R)-5,7-dihydroxy-2-(4-hydroxyphenyl)chroman-4-one	42.36	0.21
	MOL002712	6-Hydroxykaempferol	62.13	0.27
	MOL002714	baicalein	33.52	0.21
	MOL002914	Eriodyctiol (flavanone)	41.35	0.24
	MOL005922	Acanthoside B	43.35	0.77
	MOL007963	1-hydroxy-2,3,5-trimethoxy-xanthone	101.06	0.30
	MOL007984	$\Delta^5,22$ -stigmastadien-3-ol	43.83	0.76
F. Suspensa	MOL000006	luteolin	36.16	0.25
	MOL000098	quercetin	46.43	0.28
	MOL000173	wogonin	30.68	0.23
	MOL000211	Mairin	55.38	0.78
	MOL000358	beta-sitosterol	36.91	0.75
	MOL000422	kaempferol	41.88	0.24
	MOL000522	arctiin	34.45	0.84
	MOL000791	bicuculline	69.67	0.88
	MOL003281	20(S)-dammar-24-ene-3 β ,20-diol-3-acetate	40.23	0.82
	MOL003283	(2R,3R,4S)-4-(4-hydroxy-3-methoxyphenyl)-7-methoxy-2,3-dimethylol-tetralin-6-ol	66.51	0.39
	MOL003290	(3R,4R)-3,4-bis[(3,4-dimethoxyphenyl)methyl]oxolan-2-one	52.30	0.48
	MOL003295	(+)-pinoresinol monomethyl ether	53.08	0.57
	MOL003305	PHILLYRIN	36.40	0.86
	MOL003306	ACon1_001697	85.12	0.57
	MOL003308	(+)-pinoresinol monomethyl ether-4-D-beta-glucoside Qt	61.20	0.57
	MOL003315	3beta-Acetyl-20,25-epoxydammarane-24alpha-ol	33.07	0.79

	MOL003322	FORSYTHINOL	81.25	0.57
	MOL003330	(-)-Phillygenin	95.04	0.57
	MOL003344	β -amyrin acetate	42.06	0.74
	MOL003347	hyperforin	44.03	0.60
	MOL003348	adhyperforin	44.03	0.61
	MOL003365	Lactucasterol	40.99	0.85
	MOL003370	Onjixanthone I	79.16	0.30
P. Cuspidatum	MOL000006	luteolin	36.16	0.25
	MOL000098	quercetin	46.43	0.28
	MOL000358	beta-sitosterol	36.91	0.75
	MOL000492	(+)-catechin	54.83	0.24
	MOL002259	Physciondiglucoside	41.65	0.63
	MOL002268	rhein	47.07	0.28
	MOL002280	Torachryson-8-O-beta-D-(6'-oxayl)-glucoside	43.02	0.74
	MOL013281	6,8-Dihydroxy-7-methoxyxanthone	35.83	0.21
	MOL013287	Physovenine	106.21	0.19
	MOL013288	Picalinal	58.01	0.75
P. Ginseng	MOL000358	beta-sitosterol	36.91	0.75
	MOL000422	kaempferol	41.88	0.24
	MOL000449	Stigmasterol	43.83	0.76
	MOL000787	Fumarine	59.26	0.83
	MOL002879	Diop	43.59	0.39
	MOL003648	Inermin	65.83	0.54
	MOL004492	Chrysanthemaxanthin	38.72	0.58
	MOL005308	Aposiopolamine	66.65	0.22
	MOL005314	Celabenzine	101.88	0.49
	MOL005317	Deoxyharringtonine	39.27	0.81
	MOL005318	Dianthramine	40.45	0.20
	MOL005320	arachidonate	45.57	0.20
	MOL005321	Frutinone A	65.90	0.34
	MOL005344	ginsenoside rh2	36.32	0.56
	MOL005348	Ginsenoside-Rh4_qt	31.11	0.78
	MOL005356	Girinimbin	61.22	0.31
	MOL005357	Gomisin B	31.99	0.83
	MOL005360	malkangunin	57.71	0.63
	MOL005376	Panaxadiol	33.09	0.79
	MOL005384	suchilactone	57.52	0.56
	MOL005399	alexandrin_qt	36.91	0.75
	MOL005401	ginsenoside Rg5_qt	39.56	0.79

R. Tanguticum	MOL000096	(-)-catechin	49.68	0.24
	MOL000358	beta-sitosterol	36.91	0.75
	MOL000471	aloe-emodin	83.38	0.24
	MOL000554	gallic		
		acid-3-O-(6'-O-galloyl)-glucoside	30.25	0.67
	MOL002235	EUPATIN	50.80	0.41
	MOL002251	Mutatochrome	48.64	0.61
	MOL002259	Physciondiglucoside	41.65	0.63
	MOL002260	Procyanidin B-5,3'-O-gallate	31.99	0.32
	MOL002268	rhein	47.07	0.28
	MOL002276	Sennoside E_qt	50.69	0.61
	MOL002280	Torachryson-8-O-beta-D-(6'-oxayl)-glucoside	43.02	0.74
		Toralactone	46.46	0.24
	MOL002288	Emodin-1-O-beta-D-glucopyranoside	44.81	0.80
	MOL002293	Sennoside D_qt	61.06	0.61
	MOL002297	Daucosterol_qt	35.89	0.70
	MOL002303	palmidin A	32.45	0.65
S. Baicalensis	MOL000173	wogonin	30.68	0.23
	MOL000228	(2R)-7-hydroxy-5-methoxy-2-phenylchroman-4-one	55.23	0.20
		beta-sitosterol	36.91	0.75
	MOL000358	beta-sitosterol	36.91	0.75
	MOL000359	sitosterol	36.91	0.75
	MOL000525	Norwogonin	39.40	0.21
	MOL000552	5,2'-Dihydroxy-6,7,8-trimethoxyflavone	31.71	0.35
		acacetin	34.97	0.24
	MOL001689	acacetin	34.97	0.24
	MOL002714	baicalein	33.52	0.21
	MOL002908	5,8,2'-Trihydroxy-7-methoxyflavone	37.01	0.27
		5,7,2,5-tetrahydroxy-8,6-dimethoxyflavone	33.82	0.45
	MOL002910	Carthamidin	41.15	0.24
	MOL002911	2,6,2',4'-tetrahydroxy-6'-methoxychalcone	69.04	0.22
		Dihydrobaicalin_qt	40.04	0.21
MOL002914	Eriodyctiol (flavanone)	41.35	0.24	
MOL002915	Salvigenin	49.07	0.33	

	MOL002917	5,2',6'-Trihydroxy-7,8-dimethoxyflavone	45.05	0.33
	MOL002925	5,7,2',6'-Tetrahydroxyflavone	37.01	0.24
	MOL002926	dihydrooroxylin A	38.72	0.23
	MOL002927	Skullcapflavone II	69.51	0.44
	MOL002928	oroxylin a	41.37	0.23
	MOL002932	Panicolin	76.26	0.29
	MOL002933	5,7,4'-Trihydroxy-8-methoxyflavone	36.56	0.27
	MOL002934	NEOBAICALEIN	104.34	0.44
	MOL002937	DIHYDROOROXYLIN	66.06	0.23
S. Miltiorrhiza	MOL000006	luteolin	36.16	0.25
	MOL000569	digallate	61.85	0.26
	MOL001601	1,2,5,6-tetrahydrotanshinone	38.75	0.36
	MOL001659	Poriferasterol	43.83	0.76
	MOL001771	poriferast-5-en-3beta-ol	36.91	0.75
	MOL001942	isoimperatorin	45.46	0.23
	MOL002222	sugiol	36.11	0.28
	MOL002651	Dehydrotanshinone II A	43.76	0.40
	MOL002776	Baicalin	40.12	0.75
	MOL006824	α -amyrin	39.51	0.76
	MOL007036	5,6-dihydroxy-7-isopropyl-1,1-dimethyl-2,3-dihydrophenanthrene-4-one	33.77	0.29
	MOL007041	2-isopropyl-8-methylphenanthrene-3,4-dione	40.86	0.23
	MOL007045	3 α -hydroxytanshinone II a	44.93	0.44
	MOL007048	(E)-3-[2-(3,4-dihydroxyphenyl)-7-hydroxy-benzofuran-4-yl]acrylic acid	48.24	0.31
	MOL007049	4-methylenemiltirone	34.35	0.23
	MOL007050	2-(4-hydroxy-3-methoxyphenyl)-5-(3-hydroxypropyl)-7-methoxy-3-benzofurancarboxaldehyde	62.78	0.40
	MOL007051	6-o-syringyl-8-o-acetylshanzhiside methyl ester	46.69	0.71
	MOL007058	formyltanshinone	73.44	0.42
	MOL007059	3-beta-Hydroxymethylenetanshinone	32.16	0.41
	MOL007061	Methylenetanshinone	37.07	0.36

MOL007063	przewalskin a	37.11	0.65
MOL007064	przewalskin b	110.32	0.44
MOL007068	Przewaquinone B	62.24	0.41
MOL007069	przewaquinone c	55.74	0.40
MOL007070	(6S,7R)-6,7-dihydroxy-1,6-dimethyl-8,9-dihydro-7H-naphtho[8,7-g]benzofuran-10,11-dione	41.31	0.45
MOL007071	przewaquinone f	40.31	0.46
MOL007077	sclareol	43.67	0.21
MOL007079	tanshinaldehyde	52.47	0.45
MOL007081	Danshenol B	57.95	0.56
MOL007082	Danshenol A	56.97	0.52
MOL007085	Salvilenone	30.38	0.38
MOL007088	cryptotanshinone	52.34	0.40
MOL007093	dan-shexinkum d	38.88	0.55
MOL007094	danshenspiroketallactone	50.43	0.31
MOL007098	deoxyneocryptotanshinone	49.40	0.29
MOL007100	dihydrotanshinlactone	38.68	0.32
MOL007101	dihydrotanshinone I	45.04	0.36
MOL007105	epidanshenspiroketallactone	68.27	0.31
MOL007107	C09092	36.07	0.25
MOL007108	isocryptotanshinone	54.98	0.39
MOL007111	Isotanshinone II	49.92	0.40
MOL007115	manool	45.04	0.20
MOL007118	microstegiol	39.61	0.28
MOL007119	miltionone I	49.68	0.32
MOL007120	miltionone II	71.03	0.44
MOL007121	miltipolone	36.56	0.37
MOL007122	Miltirone	38.76	0.25
MOL007123	miltirone II	44.95	0.24
MOL007124	neocryptotanshinone ii	39.46	0.23
MOL007125	neocryptotanshinone	52.49	0.32
MOL007127	1-methyl-8,9-dihydro-7H-naphtho[5,6-g]benzofuran-6,10,11-trione	34.72	0.37
MOL007130	prolithospermic acid	64.37	0.31
MOL007132	(2R)-3-(3,4-dihydroxyphenyl)-2-[(Z)-3-(3,4-dihydroxyphenyl)acryloyl]oxy-propionic acid	109.38	0.35

MOL007140	(Z)-3-[2-[(E)-2-(3,4-dihydroxyphenyl)vinyl]-3,4-dihydroxyphenyl]acrylic acid	88.54	0.26
MOL007141	salvianolic acid g	45.56	0.61
MOL007142	salvianolic acid j	43.38	0.72
MOL007143	salvilenone l	32.43	0.23
MOL007145	salviolone	31.72	0.24
MOL007149	NSC 122421	34.49	0.28
MOL007150	(6S)-6-hydroxy-1-methyl-6-methylol-8,9-dihydro-7H-naphtho[8,7-g]benzofuran-10,11-quinone	75.39	0.46
MOL007151	Tanshindiol B	42.67	0.45
MOL007152	Przewaquinone E	42.85	0.45
MOL007154	tanshinone iia	49.89	0.40
MOL007155	(6S)-6-(hydroxymethyl)-1,6-dimethyl-8,9-dihydro-7H-naphtho[8,7-g]benzofuran-10,11-dione	65.26	0.45
MOL007156	tanshinone VI	45.64	0.30

Footnotes: OB (oral bioavailability); DL: drug likeness.

Table S2. The information about the enrolled medical plants.

Herb name	References	Enrolled Compound Number
S. Miltiorrhiza	PMID: 15553818 PMID: 21134421	65
S. Baicalensis	PMID: 30686973 PMID: 30127597	24
F. Suspensa	PMID: 31923823	23
P. Ginseng	PMID: 24052247 PMID: 15832003	22
A. Annua	PMID: 30108544	22
C. Tinctorius	PMID: 27599591	22
A. Bidentatae	PMID: 34790728	20
C. Monnieri	PMID: 22153917	19
D. Fortune	PMID: 36565356	18
R. Tanguticum	PMID: 27901023 PMID: 28264680	16
E. Breviscapus	PMID: 28250753	12
P. Cuspidatum	PMID: 27122047 PMID: 18654909	10
C. Sativus	PMID: 35322143	5
C. Longa	PMID: 23932920	3
C. Asiatica	PMID: 34924122	3
C. Zedoaria	PMID: 29992051	3

Table S3. The top 15 central proteins in the protein-protein network of the compound targets.

Proteins	BetweennessCentrality	Proteins	Degree
AR	0.01680068	CYP19A1	165
CDK2	0.01405804	AR	165
ESR2	0.01348334	ESR2	160
ESR1	0.01345255	ACHE	159
GSK3B	0.01334269	ESR1	152
CYP19A1	0.01269389	CDK2	142
KDR	0.01234043	PTGS2	139
EGFR	0.01123543	AKR1B1	136
PTGS2	0.01119334	GSK3B	131
ACHE	0.01068041	KDR	129
MAPK14	0.01024397	NOS2	123
MAPK8	0.0098862	CDK1	120
PARP1	0.00933457	EGFR	118
PIM1	0.00831	MAPK14	117
PDE10A	0.00810412	ADORA1	115

Table S4. The details of topologic analysis of the overlapped targets of compound and TBI by Cytohubba.

Node name	MCC	DMNC	MNC	Degree	EPC	Bottle Neck	EcCentricity	Closeness	Radiality	Betweenness	Stress	Clustering Coefficient
AKT1	2.51E+13	0.49	87	87	26.03	75	0.33	106.33	3.72	1657.35	13360	0.26
IL6	4.76E+13	0.57	75	76	25.37	3	0.33	100.33	3.61	1120.96	9090	0.31
VEGFA	4.76E+13	0.56	75	75	24.76	2	0.33	100.00	3.61	893.44	8192	0.31
TNF	4.76E+13	0.61	67	67	23.85	1	0.33	95.83	3.54	553.65	5804	0.35
CASP3	4.76E+13	0.59	64	64	22.69	3	0.33	94.67	3.53	702.54	6178	0.35
SRC	4.76E+13	0.62	62	63	23.98	7	0.33	94.17	3.52	920.20	7886	0.35
EGFR	4.75E+13	0.61	60	60	22.57	4	0.33	92.00	3.47	508.12	5298	0.36
APP	1.36E+12	0.55	58	58	21.45	7	0.50	92.00	3.50	797.27	6712	0.33
STAT3	4.76E+13	0.67	55	55	22.12	1	0.33	90.00	3.45	389.75	4278	0.41
PTGS2	4.60E+13	0.69	54	54	22.03	1	0.33	89.17	3.43	345.35	3664	0.43
KNG1	1.31E+12	0.58	51	51	19.89	10	0.33	87.83	3.41	659.09	6514	0.36
CXCR4	4.77E+13	0.72	50	50	21.79	1	0.33	87.17	3.40	284.03	3232	0.46
TLR4	4.67E+11	0.67	49	49	20.89	2	0.33	86.67	3.39	414.02	4128	0.42
MTOR	4.69E+13	0.73	45	45	19.32	1	0.33	84.83	3.37	255.67	2564	0.48
NOS3	5.27E+11	0.63	43	43	19.14	1	0.33	83.50	3.33	278.58	2874	0.42
CCND1	4.67E+13	0.78	41	41	18.29	1	0.33	82.33	3.31	114.91	1306	0.53
KDR	4.68E+13	0.75	39	39	19.01	3	0.33	81.50	3.30	340.07	3450	0.52
ESR1	4.74E+13	0.88	38	38	19.46	1	0.33	80.67	3.28	71.25	956	0.60
SIRT1	4.40E+11	0.77	37	37	17.88	3	0.33	80.17	3.27	114.69	1208	0.54
HIF1A	4.54E+13	0.79	37	37	18.81	1	0.33	80.17	3.27	99.30	1196	0.55
SERPINE1	5.29E+11	0.78	36	36	18.02	1	0.33	79.83	3.27	116.05	1486	0.55
STAT1	4.36E+13	0.77	35	35	17.08	1	0.33	79.17	3.25	113.67	1336	0.54
ERBB2	4.50E+13	0.78	34	34	17.73	4	0.33	78.33	3.23	268.96	2464	0.56

F2	4.28E+09	0.67	34	34	17.09	3	0.33	79.00	3.26	198.20	2626	0.48
OPRM1	1.31E+12	0.70	32	33	15.51	2	0.33	78.83	3.27	352.74	4566	0.48
SELP	1.50E+09	0.72	30	30	16.06	1	0.33	76.67	3.21	86.56	1128	0.54
CNR1	1.31E+12	0.70	29	29	14.00	2	0.33	76.00	3.20	167.72	2582	0.52
PLG	4.10E+11	0.86	29	29	16.39	1	0.33	76.17	3.21	107.26	1542	0.65
AGTR1	1.56E+09	0.71	29	29	15.91	1	0.33	76.50	3.22	77.68	1226	0.53
CXCR2	1.31E+12	0.86	29	29	16.06	1	0.33	76.17	3.21	48.12	964	0.65
MAPK10	4.37E+10	0.72	27	28	14.93	2	0.33	75.67	3.20	345.74	2686	0.51
GRM5	3.77E+06	0.46	28	28	12.05	5	0.33	75.17	3.17	337.88	2890	0.35
HMOX1	2.10E+10	0.80	27	28	15.29	2	0.33	75.50	3.19	311.78	2526	0.57
NFKB1	5.61E+11	0.94	28	28	15.86	1	0.33	75.00	3.17	23.29	342	0.71
ADRBK1	4.86E+08	0.62	27	27	13.47	1	0.33	75.17	3.19	115.74	1266	0.48
TXN	1.37E+11	0.79	27	27	14.64	1	0.25	74.58	3.16	54.29	622	0.61
BDKRB2	1.31E+12	0.74	26	26	12.58	1	0.33	72.33	3.07	47.51	564	0.58
CCR1	1.31E+12	0.87	26	26	14.45	1	0.33	74.50	3.17	37.10	736	0.68
CXCR3	1.31E+12	0.89	26	26	14.97	1	0.33	74.50	3.17	33.96	692	0.70
FLT1	2.12E+13	0.92	26	26	15.42	1	0.33	74.33	3.17	21.71	356	0.72
ADCY1	1.31E+12	0.67	22	25	11.47	3	0.33	73.00	3.12	389.48	2394	0.43
ENSG000001 96689	7.73E+06	0.58	25	25	13.70	1	0.33	74.67	3.20	142.89	2500	0.46
ADORA1	1.31E+12	0.87	25	25	13.13	1	0.33	74.17	3.17	33.35	610	0.69
TLR9	3.76E+10	0.87	25	25	14.61	1	0.25	73.08	3.12	23.49	338	0.69
P2RY12	1.31E+12	0.80	23	23	12.57	1	0.33	72.50	3.13	35.75	438	0.66
PRKCZ	2.03E+08	0.69	22	22	13.47	1	0.33	72.83	3.16	51.04	638	0.58
PDGFRB	1.31E+12	0.77	22	22	13.60	1	0.33	72.00	3.12	29.03	398	0.64
GSK3B	1.29E+10	0.79	22	22	13.02	1	0.33	72.00	3.12	23.37	288	0.66
C5AR1	1.31E+12	0.87	22	22	12.61	1	0.33	71.67	3.10	21.33	356	0.72

HDAC1	2.81E+11	0.87	22	22	14.21	1	0.25	70.92	3.06	20.67	244	0.72
BDKRB1	1.31E+12	0.86	22	22	11.17	1	0.33	69.67	3.01	19.54	224	0.71
SHH	2.00E+09	0.81	20	21	13.28	1	0.33	71.83	3.13	117.30	1196	0.63
FPR1	1.31E+12	0.85	21	21	11.70	1	0.33	70.67	3.07	20.83	314	0.71
ADORA3	1.31E+12	0.97	21	21	12.56	1	0.33	72.17	3.14	12.58	386	0.82
CDK5	1.43E+05	0.60	20	20	12.23	1	0.33	71.33	3.12	42.30	504	0.51
MMP7	1.58E+12	0.99	20	20	14.15	1	0.33	71.33	3.12	5.89	96	0.85
NOS1	8.13E+05	0.58	19	19	11.92	1	0.33	70.83	3.11	50.01	644	0.51
EDNRB	3.68E+06	0.64	19	19	10.97	1	0.33	70.50	3.10	41.84	600	0.56
IKBKB	1.87E+10	0.85	19	19	12.16	1	0.33	70.33	3.09	15.04	228	0.74
F3	2.51E+08	0.85	19	19	11.90	1	0.33	70.33	3.09	14.74	240	0.74
TERT	2.54E+10	0.92	19	19	12.56	1	0.33	70.17	3.08	8.89	130	0.81
MET	1.32E+12	1.03	18	18	13.40	1	0.33	70.33	3.10	2.20	48	0.92
GRIN1	7.82E+02	0.40	17	17	7.45	1	0.33	69.50	3.08	170.92	1814	0.36
NLRP3	2.10E+08	0.85	17	17	12.36	1	0.25	68.92	3.05	10.09	158	0.77
PKM	7.68E+05	0.62	16	16	9.60	2	0.25	68.58	3.05	142.55	1442	0.58
LGALS3	1.17E+07	0.78	16	16	11.03	2	0.33	67.83	3.02	58.62	608	0.73
PTGER4	3.99E+06	0.63	16	16	11.09	1	0.33	69.17	3.08	35.02	436	0.58
ADAM10	3.06E+04	0.56	16	16	10.65	2	0.33	69.00	3.07	29.39	346	0.52
TACR1	3.68E+06	0.70	16	16	9.63	1	0.33	69.17	3.08	25.33	586	0.65
MAP3K5	6.17E+06	0.76	16	16	11.87	1	0.33	69.00	3.07	24.95	240	0.71
IDO1	5.08E+07	0.76	16	16	11.59	1	0.25	68.92	3.06	20.27	242	0.71
ITGB3	8.30E+04	0.66	16	16	9.81	1	0.33	68.50	3.05	18.33	228	0.62
ESR2	1.48E+09	0.92	16	16	11.38	1	0.25	68.58	3.05	5.40	76	0.86
GRIN2A	7.86E+02	0.47	15	15	7.23	1	0.33	68.83	3.08	83.12	1082	0.45
IDH1	4.80E+03	0.56	15	15	9.01	1	0.33	66.67	2.98	69.01	626	0.53
NGFR	3.11E+04	0.66	14	15	9.42	1	0.33	68.00	3.04	29.19	332	0.56

MAPT	9.12E+04	0.64	15	15	9.30	1	0.33	69.17	3.10	26.52	292	0.61
TBXA2R	3.63E+06	0.59	15	15	7.65	1	0.33	66.33	2.96	23.53	212	0.56
MME	3.53E+03	0.54	15	15	10.07	1	0.33	68.00	3.04	15.92	240	0.51
FGFR1	1.60E+08	0.90	15	15	10.79	1	0.33	67.67	3.02	4.33	66	0.86
NTRK1	4.76E+02	0.43	14	14	8.10	1	0.33	67.33	3.02	75.33	1042	0.42
ADORA2A	9.67E+04	0.68	14	14	9.88	1	0.33	68.67	3.09	16.56	238	0.66
PRKCE	3.76E+02	0.41	11	13	6.80	1	0.33	66.83	3.02	53.93	700	0.31
PLA2G1B	3.67E+06	0.74	13	13	8.64	1	0.33	66.83	3.02	10.69	184	0.74
SIRT2	1.14E+04	0.65	13	13	9.19	1	0.33	66.67	3.01	9.02	130	0.65
LRRK2	2.07E+03	0.56	12	12	7.51	1	0.33	66.00	2.99	42.95	522	0.58
MIF	4.45E+05	0.82	12	12	9.16	1	0.25	65.75	2.98	2.50	44	0.85
G6PD	1.92E+03	0.58	11	11	6.46	1	0.25	64.75	2.94	74.18	800	0.62
TRPA1	5.08E+02	0.46	11	11	5.55	1	0.25	59.75	2.70	18.19	138	0.49
PLA2G4A	6.02E+03	0.63	11	11	7.95	1	0.25	65.42	2.98	6.23	74	0.67
BCL2A1	2.09E+04	0.71	11	11	8.03	1	0.25	64.75	2.94	5.39	56	0.76
SCN10A	2.58E+02	0.40	10	10	5.32	2	0.33	63.17	2.89	202.74	2068	0.44
MAOB	5.90E+01	0.33	9	10	5.34	1	0.33	63.17	2.89	82.82	750	0.31
PTGIR	5.20E+01	0.38	10	10	5.50	1	0.33	62.17	2.84	15.53	110	0.42
HSF1	1.68E+03	0.62	9	10	6.67	1	0.25	63.58	2.90	11.30	70	0.58
EGLN1	2.40E+03	0.66	10	10	7.64	1	0.25	64.25	2.94	3.46	52	0.73
ITGAV	1.81E+03	0.62	10	10	7.30	1	0.25	62.75	2.87	2.90	32	0.69
IGFBP5	4.06E+04	0.72	10	10	7.74	1	0.33	65.17	2.98	1.69	26	0.80
AXL	3.63E+05	0.78	10	10	8.62	1	0.25	64.92	2.97	1.40	18	0.87
GRIK2	1.32E+02	0.48	9	9	3.87	1	0.25	60.75	2.79	46.77	412	0.56
PDE5A	1.45E+03	0.57	9	9	6.89	1	0.25	63.92	2.94	7.48	148	0.67
PPIA	2.28E+03	0.69	9	9	6.86	1	0.25	62.92	2.89	1.25	22	0.81
SLC1A3	5.40E+01	0.35	8	8	4.32	2	0.25	60.75	2.80	33.15	262	0.43

ECE1	5.60E+01	0.52	6	8	5.48	1	0.33	63.50	2.94	9.47	124	0.39
F7	5.06E+03	0.70	8	8	5.63	1	0.25	61.58	2.84	5.09	92	0.86
SCN2A	2.80E+01	0.57	4	7	3.23	2	0.25	57.25	2.64	79.17	764	0.38
CAMK4	1.90E+01	0.38	6	7	4.13	1	0.33	60.83	2.83	10.68	116	0.38
GLRA1	9.60E+01	0.55	7	7	3.23	1	0.25	54.25	2.50	9.91	130	0.71
TRPM8	3.60E+02	0.66	7	7	4.07	1	0.25	56.33	2.60	1.48	16	0.86
F13A1	1.44E+03	0.73	7	7	6.57	1	0.33	62.17	2.89	0.10	2	0.95
GLP1R	3.00E+01	0.48	6	6	5.37	1	0.25	61.92	2.89	3.53	78	0.67
MAPKAPK2	3.20E+01	0.43	6	6	5.43	1	0.33	61.67	2.88	2.55	30	0.60
CASP2	7.20E+01	0.57	6	6	5.30	1	0.25	60.75	2.83	0.90	6	0.80
GC	2.50E+01	0.57	4	5	3.89	1	0.25	54.67	2.56	9.07	64	0.60
IL6ST	2.50E+01	0.57	4	5	4.20	1	0.25	59.08	2.76	1.10	12	0.60
GRIK1	4.80E+01	0.58	5	5	2.30	1	0.25	49.92	2.31	0.48	4	0.90
SLC18A2	4.00E+00	0.31	2	4	2.78	1	0.25	53.42	2.52	3.87	38	0.17
PTPRS	8.00E+00	0.38	4	4	3.64	1	0.25	57.75	2.72	0.74	10	0.67
AKR1A1	3.00E+00	0.31	2	3	1.87	1	0.25	47.42	2.21	3.35	10	0.33
CYP27B1	2.00E+00	0.00	1	2	2.35	1	0.25	55.50	2.63	2.84	64	0.00
CACNA2D1	2.00E+00	0.31	2	2	1.22	1	0.25	43.17	1.96	0.00	0	1.00
PEPD	2.00E+00	0.31	2	2	2.07	1	0.25	48.92	2.30	0.00	0	1.00
MERTK	2.00E+00	0.31	2	2	2.08	1	0.25	51.42	2.44	0.00	0	1.00
PDE1A	1.00E+00	0.00	1	1	1.43	1	0.25	45.42	2.13	0.00	0	0.00
CHRNA	1.00E+00	0.00	1	1	1.74	1	0.25	52.83	2.53	0.00	0	0.00
EPHX1	1.00E+00	0.00	1	1	1.63	1	0.25	46.42	2.20	0.00	0	0.00
MAP3K12	1.00E+00	0.00	1	1	1.52	1	0.25	46.50	2.21	0.00	0	0.00

Footnotes: MCC:Maximal Clique Centrality; MNC:Maximum Neighborhood Component; EPC: Edge Percolated Component; DMNC: Density of Maximum Neighborhood Component.

Table S5. Molecular docking details of EGFR to the putative ligands.

Mol ID	Molecule Name	PubChem_ID	Docking Score
MOL005314	Celabenzine	442847	-8.7
MOL000006	luteolin	5280445	-8.4
MOL002776	Baicalin	64982	-8.4
MOL005344	ginsenoside rh2	119307	-8.3
MOL002293	Sennoside D qt	135397905	-8.3
MOL002925	5,7,2',6'-Tetrahydroxyflavone	5321865	-8.2
MOL002933	5,7,4'-Trihydroxy-8-methoxyflavone	5322078	-8.2
MOL005376	Panaxadiol	73498	-8.1
MOL007401	Cirsiliol	160237	-8.1
MOL001689	acacetin	5280442	-8.1
MOL002881	Diosmetin	5281612	-8.1
MOL000525	Norwogonin	5281674	-8.1
MOL002280	Torachryson-8-O-beta-D-(6'-oxayl)-glucoside	78385603	-8.1
MOL000791	bicuculline	10237	-8
MOL002908	5,8,2'-Trihydroxy-7-methoxyflavone	156992	-8
MOL000173	wogonin	5281703	-8
MOL009091	xanthogalenol	14309735	-8
MOL005356	Girinimbin	96943	-7.9
MOL002259	Physciondiglucoside	442762	-7.9
MOL001978	Aureusidin	5281220	-7.9
MOL007105	epidanshenspiroketalactone	102004791	-7.9
MOL000940	bisdemethoxycurcumin	5315472	-7.8
MOL007274	Skrofulein	188323	-7.7
MOL002714	baicalein	5281605	-7.7
MOL007093	dan-shexinkum d	124307626	-7.7
MOL001601	1,2,5,6-tetrahydrotanshinone	124416	-7.6
MOL004609	Areapillin	158311	-7.6
MOL000354	isorhamnetin	5281654	-7.6
MOL007120	miltionone II	5319836	-7.6
MOL002928	oroxylin a	5320315	-7.6
MOL000392	formononetin	5280378	-7.5
MOL007101	dihydrotanshinoneI	40785034	-7.5
MOL000522	arctiin	100528	-7.4
MOL007061	Methylenetanshinquinone	105118	-7.4
MOL002651	Dehydrotanshinone II A	128994	-7.4
MOL000098	quercetin	5280343	-7.4

MOL002721	quercetagetin	5281680	-7.4
MOL004083	Tamarixetin	5281699	-7.4
MOL003305	PHILLYRIN	101712	-7.3
MOL007041	2-isopropyl-8-methylphenanthrene-3,4-dione	135872	-7.3
MOL005317	Deoxyharringtonine	285342	-7.3
MOL000422	kaempferol	5280863	-7.3
MOL002712	6-Hydroxykaempferol	5281638	-7.3
MOL004112	Patuletin	5281678	-7.3
MOL007050	2-(4-hydroxy-3-methoxyphenyl)-5-(3-hydroxypropyl)-7-methoxy-3-benzofurancarboxaldehyde	6709746	-7.3
MOL007132	(2R)-3-(3,4-dihydroxyphenyl)-2-[(Z)-3-(3,4-dihydroxyphenyl)acryloyl]oxy-propionic acid	9841799	-7.3
MOL002694	4-[(E)-4-(3,5-dimethoxy-4-oxo-1-cyclohexa-2,5-dienylidene)but-2-enylidene]-2,6-dimethoxycyclohexa-2,5-dien-1-one	10237057	-7.3
MOL002915	Salvigenin	161271	-7.2
MOL002932	Panicolin	5320399	-7.2
MOL007141	salvianolic acid g	11530200	-7.2
MOL007058	formyltanshinone	14609847	-7.2
MOL005308	Aposiopolamine	101612220	-7.2
MOL007424	artemisinin	68827	-7.1
MOL000552	5,2'-Dihydroxy-6,7,8-trimethoxyflavone	159029	-7.1
MOL007082	Danshenol A	3083514	-7.1
MOL002235	EUPATIN	5317287	-7.1
MOL007069	przewaquinone c	126071	-6.9
MOL007155	(6S)-6-(hydroxymethyl)-1,6-dimethyl-8,9-dihydro-7H-naphtho[8,7-g]benzofuran-10,11-dione	9926694	-6.9
MOL002268	rhein	10168	-6.8
MOL007156	tanshinone VI	149138	-6.8
MOL007412	DMQT	5281603	-6.8
MOL003605	(E)-2,3-bis(2-keto-7-methoxy-chromen-8-yl)acrolein	10597338	-6.8
MOL003607	cniforin B	58488745	-6.8
MOL003584	Xanthoxylin N	66548	-6.7

MOL007425	dihydroartemisinin	3000518	-6.7
MOL002917	5,2',6'-Trihydroxy-7,8-dimethoxyflavone	5322059	-6.7
MOL007077	scclareol	7060889	-6.7
MOL003370	Onjixanthone I	5320290	-6.5
MOL005357	Gomisin B	6438572	-6.5
MOL003606	cniforin A	15553295	-6.5
MOL002927	Skullcapflavone II	124211	-6.4
MOL002909	5,7,2,5-tetrahydroxy-8,6-dimethoxyflavone	44258628	-6.4
MOL005229	Artemetin	5320351	-6.2
MOL013287	Physovenine	442113	-6.1
MOL001389	n-heptanal	8130	-4.3
