

Supplementary

Table S1 The active components of CHSGS

TCM	Mol ID	Molecule Name
Chaihu	MOL001645	Linoleyl acetate
Chaihu	MOL002776	Baicalin
Chaihu	MOL000449	Stigmasterol
Chaihu	MOL000354	isorhamnetin
Chaihu	MOL000422	kaempferol
Chaihu	MOL004598	3,5,6,7-tetramethoxy-2-(3,4,5-trimethoxyphenyl)chromone
Chaihu	MOL004609	Areapillin
Chaihu	MOL013187	Cubebin
Chaihu	MOL004624	Longikauringin A
Chaihu	MOL004628	Octalupine
Chaihu	MOL004644	Sainfuran
Chaihu	MOL004648	Troxerutin
Chaihu	MOL004653	(+)-Anomalin
Chaihu	MOL004702	saikosaponin c_qt
Chaihu	MOL004718	α-spinasterol
Chaihu	MOL000490	petunidin
Chaihu	MOL000098	quercetin
Baishao	MOL001910	11α,12α-epoxy-3β,23-dihydroxy-30-norolean-20-en-28,12β-olide
Baishao	MOL001918	paeoniflorigenone
Baishao	MOL001919	(3S,5R,8R,9R,10S,14S)-3,17-dihydroxy-4,4,8,10,14-pentamethyl-2,3,5,6,7,9-hexahydro-1H-cyclopenta[aj]phenanthrene-15,16-dione
Baishao	MOL001921	Lactiflorin
Baishao	MOL001924	paeoniflorin
Baishao	MOL001925	paeoniflorin_qt
Baishao	MOL001928	albiflorin_qt
Baishao	MOL001930	benzoyl paeoniflorin
Baishao	MOL000211	Mairin
Baishao	MOL000358	beta-sitosterol
Baishao	MOL000359	sitosterol
Baishao	MOL000422	kaempferol
Baishao	MOL000492	(+)-catechin
Ezhu	MOL000296	hederagenin
Ezhu	MOL000906	wenjine
Ezhu	MOL000940	bisdemethoxycurcumin
Danggui	MOL000358	beta-sitosterol
Danggui	MOL000449	Stigmasterol
Chuanxiong	MOL002135	Myricanone
Chuanxiong	MOL002140	Perfolyrine
Chuanxiong	MOL002151	senkyunone
Chuanxiong	MOL002157	wallichilide
Chuanxiong	MOL000359	sitosterol
Chuanxiong	MOL000433	FA
Yujin	MOL000358	beta-sitosterol
Yujin	MOL000359	sitosterol
Yujin	MOL004241	curculactone
Yujin	MOL004244	(4aR,5R,8R,8aR)-5,8-dihydroxy-3,5,8a-trimethyl-6,7,8,9-tetrahydro-4aH-benzof[benzofuran-4-one
Yujin	MOL004253	Curcumenolactone C
Yujin	MOL004260	(E)-1,7-Diphenyl-3-hydroxy-1-hepten-5-one
Yujin	MOL004263	(E)-5-Hydroxy-7-(4-hydroxyphenyl)-1-phenyl-1-heptene
Yujin	MOL004291	Oxycurcumenol
Yujin	MOL004305	Zedoalactone A
Yujin	MOL004306	Zedoalactone B
Yujin	MOL004309	zedoalactone E
Yujin	MOL004311	Zedoarolide A
Yujin	MOL004313	Zedoarolide B
Yujin	MOL004316	1,7-Diphenyl-3-acetoxy-6(E)-hepten
Yujin	MOL004328	naringenin
Xiangfu	MOL003044	Chryseriol
Xiangfu	MOL000354	isorhamnetin
Xiangfu	MOL003542	8-Isopentenyl-kaempferol
Xiangfu	MOL000358	beta-sitosterol
Xiangfu	MOL000359	sitosterol
Xiangfu	MOL004027	1,4-Epoxy-16-hydroxyheneicos-1,3,12,14,18-pentaene
Xiangfu	MOL004053	Isodalbergin
Xiangfu	MOL004058	Khell
Xiangfu	MOL004059	khellol glucoside
Xiangfu	MOL010489	Resivit
Xiangfu	MOL004068	rosenonolactone
Xiangfu	MOL004071	Hyndarin
Xiangfu	MOL004074	stigmasterol glucoside_qt
Xiangfu	MOL004077	sugeonyl acetate
Xiangfu	MOL000422	kaempferol
Xiangfu	MOL000449	Stigmasterol
Xiangfu	MOL000006	luteolin
Xiangfu	MOL000098	quercetin
Dihuang	MOL000359	sitosterol
Dihuang	MOL000449	Stigmasterol
Zhimu	MOL001677	asperglaucide
Zhimu	MOL003773	Mangiferolic acid
Zhimu	MOL000422	kaempferol
Zhimu	MOL004373	Anhydrocaritin
Zhimu	MOL004489	Anemarsaponin F_qt
Zhimu	MOL004492	Chrysanthemaxanthin
Zhimu	MOL004497	Hippeastrine
Zhimu	MOL004514	Timosaponin B III_qt
Zhimu	MOL000449	Stigmasterol
Zhimu	MOL004528	Icarin I
Zhimu	MOL004540	Anemarsaponin C_qt
Zhimu	MOL004542	Anemarsaponin E_qt
Zhimu	MOL000483	(Z)-3-(4-hydroxy-3-methoxy-phenyl)-N-[2-(4-hydroxyphenyl)ethyl]acrylamide
Zhimu	MOL000546	diosgenin
Zhimu	MOL000631	coumaroyltyramine
Banzhilian	MOL001755	24-Ethylcholest-4-en-3-one
Banzhilian	MOL002714	baicalein
Banzhilian	MOL002719	6-Hydroxynaringenin
Banzhilian	MOL002915	Salvigenin
Banzhilian	MOL000351	Rhamnazin
Banzhilian	MOL000359	sitosterol
Banzhilian	MOL005190	eriodictyol
Banzhilian	MOL005869	daucostero_qt
Banzhilian	MOL000006	luteolin
Banzhilian	MOL008206	Moslosooflavone
Banzhilian	MOL000098	quercetin
Mihoutaogen	MOL000358	beta-sitosterol
Mihoutaogen	MOL000359	sitosterol
Mihoutaogen	MOL000471	aloe-emodin
Mihoutaogen	MOL000492	(+)-catechin
Mihoutaogen	MOL000073	ent-Epicatechin
Mihoutaogen	MOL000098	quercetin
Baihuasheshhecao	MOL001646	2,3-dimethoxy-6-methanthraquinone
Baihuasheshhecao	MOL001659	Poriferasterol
Baihuasheshhecao	MOL001663	(4aS,6aR,6aS,6bR,8aR,10R,12aR,14bS)-10-hydroxy-2,2,6a,6b,9,9,12a-heptamethyl-1,3,4,5,6,6a,7,8,8a,10,11,12,13,14b-tetradecahydronicene-4a-carboxylic acid
Baihuasheshhecao	MOL001670	2-methoxy-3-methyl-9,10-antraquinone
Baihuasheshhecao	MOL000449	Stigmasterol
Baihuasheshhecao	MOL000358	beta-sitosterol
Baihuasheshhecao	MOL000098	quercetin
Shanzhuyu	MOL001494	Mandanol
Shanzhuyu	MOL001495	Ethyl linolenate
Shanzhuyu	MOL001771	poriferast-5-en-3beta-ol
Shanzhuyu	MOL002879	Diop
Shanzhuyu	MOL002883	Ethyl oleate (NF)
Shanzhuyu	MOL003137	Leucanthoside
Shanzhuyu	MOL000358	beta-sitosterol
Shanzhuyu	MOL000359	sitosterol
Shanzhuyu	MOL000449	Stigmasterol
Shanzhuyu	MOL005360	malkangunin
Shanzhuyu	MOL005481	2,6,10,14,18-pentamethylcos-2,6,10,14,18-pentaene
Shanzhuyu	MOL005486	3,4-Dehydrolycopen-16-al
Shanzhuyu	MOL005489	3,6-Digalloylglucose
Shanzhuyu	MOL005503	Cornudentanone
Shanzhuyu	MOL005530	Hydroxygenkwanin
Shanzhuyu	MOL005531	Telocinobufganin
Shanzhuyu	MOL008457	Tetrahydroalstonine
Shanzhuyu	MOL000554	gallic acid-3-O-(6'-O-galloyl)-glucoside
Shanzhuyu	MOL005552	gemin D
Shanzhuyu	MOL005557	lanosta-8,24-dien-3-ol,3-acetate
Suanzaoren	MOL001521	ceanothic acid
Suanzaoren	MOL001522	(S)-Coclaurine
Suanzaoren	MOL001525	Daucosterol
Suanzaoren	MOL001527	jujuboside A_qt
Suanzaoren	MOL001532	phytosterol
Suanzaoren	MOL001539	sanjoinenine
Suanzaoren	MOL001542	swertisin
Suanzaoren	MOL001546	zizyphusine
Suanzaoren	MOL000211	Mairin
Tusizi	MOL001558	sesamin
Tusizi	MOL000184	NSC63551
Tusizi	MOL000354	isorhamnetin
Tusizi	MOL000358	beta-sitosterol
Tusizi	MOL000422	kaempferol
Tusizi	MOL005043	campfest-5-en-3beta-ol
Tusizi	MOL005440	isofucosterol
Tusizi	MOL005944	matrine
Tusizi	MOL006649	sophranol
Tusizi	MOL000953	CLR
Tusizi	MOL000098	quercetin
Baiziren	MOL001439	arachidonic acid
Baiziren	MOL002211	11,14-eicosadienoic acid
Baiziren	MOL000359	sitosterol
Baiziren	MOL003927	Dihomololenic acid
Baiziren	MOL008153	5Z-eicosenoic acid
Gancao	MOL001484	Inermine
Gancao	MOL001792	DFV
Gancao	MOL000211	Mairin
Gancao	MOL002311	Glycyrol
Gancao	MOL000239	Jaranol
Gancao	MOL002565	Medicarpin
Gancao	MOL000354	isorhamnetin
Gancao	MOL000359	sitosterol
Gancao	MOL003656	Lupiwighteone
Gancao	MOL003896	7-Methoxy-2-methyl isoflavone
Gancao	MOL000392	formononetin
Gancao	MOL000417	Calycosin
Gancao	MOL000422	kaempferol
Gancao	MOL004328	naringenin
Gancao	MOL004805	(2S)-2-[4-hydroxy-3-(3-methylbut-2-enyl)phenyl]-8,8-dimethyl-2,3-dihydroprano[3,2-f]chromen-4-one
Gancao	MOL004806	euchrenone
Gancao	MOL004808	glyasperin B
Gancao	MOL004810	glyasperin F
Gancao	MOL004811	Glyasperin C
Gancao	MOL004814	Isotrifolol
Gancao	MOL004815	(E)-1-(2,4-dihydroxyphenyl)-3-(2,2-dimethylchromen-6-yl)prop-2-en-1-one
Gancao	MOL004820	kanzonols W
Gancao	MOL004824	(2S)-6-(2,4-dihydroxyphenyl)-2-(2-hydroxypropan-2-yl)-4-methoxy-2,3-dihydrofuro[3,2-g]chromen-7-one
Gancao	MOL004827	Semilicoisoflavone B
Gancao	MOL004828	Glepidotin A
Gancao	MOL004829	Glepidotin B
Gancao	MOL004833	Phaseolichalavan
Gancao	MOL004835	Glypallichalcone
Gancao	MOL004838	8-(6-hydroxy-2-benzofuranyl)-2,2-dimethyl-5-chromenol
Gancao	MOL004841	Licochalcone B
Gancao	MOL004848	licochalcone G
Gancao	MOL004849	3-(2,4-dihydroxyphenyl)-8-(1,1-dimethylprop-2-enyl)-7-hydroxy-5-methoxy-coumarin
Gancao	MOL004855	Licoricone
Gancao	MOL004856	Gancaonin A
Gancao	MOL004857	Gancaonin B
Gancao	MOL004860	licorice glycoside E
Gancao	MOL004863	3-(3,4-dihydroxyphenyl)-5,7-dihydroxy-8-(3-methylbut-2-enyl)chromone
Gancao	MOL004864	5,7-dihydroxy-3-(4-methoxyphenyl)-8-(3-methylbut-2-enyl)chromone
Gancao	MOL004866	2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-6-(3-methylbut-2-enyl)chromone
Gancao	MOL004879	Glycyrin
Gancao	MOL004882	Licocoumarone
Gancao	MOL004883	Licoisoflavone
Gancao	MOL004884	Licoisoflavone B
Gancao	MOL004885	licoisoflavonone
Gancao	MOL004891	shinpterocarpin
Gancao	MOL004898	(E)-3-[3-(4-dihydroxy-5-(3-methylbut-2-enyl)phenyl)-1-(2,4-dihydroxyphenyl)prop-2-en-1-one
Gancao	MOL004903	liquiritin
Gancao	MOL004904	licopyranocoumarin
Gancao	MOL004905	3,22-Dihydroxy-11-oxo-delta(12)-oleanene-27-alpha-methoxycarbonyl-29-oic acid
Gancao	MOL004907	Glyzaglabrin
Gancao	MOL004908	Glabridin
Gancao	MOL004910	Glabranin
Gancao	MOL004911	Glabrene
Gancao	MOL004912	Glabrone
Gancao	MOL004913	1,3-dihydroxy-9-methoxy-6-benzofurano[3,2-c]chromenone
Gancao	MOL004914	1,3-dihydroxy-8,9-dimethoxy-6-benzofurano[3,2-c]chromenone
Gancao	MOL004915	Eurycarpin A
Gancao	MOL004917	glycyroside
Gancao	MOL004924	(-)-Medicocarpin
Gancao	MOL004935	Sigmoidin-B
Gancao	MOL004941	(2R)-7-hydroxy-2-(4-hydroxyphenyl)chroman-4-one
Gancao	MOL004945	(2S)-7-hydroxy-2-(4-hydroxyphenyl)-8-(3-methylbut-2-enyl)chroman-4-one
Gancao	MOL004948	Isoglycyrol
Gancao	MOL004949	Isolicoicoflavonol
Gancao	MOL004957	HMO
Gancao	MOL004959	1-Methoxyphaseollidin
Gancao	MOL004961	Quercetin der.
Gancao	MOL004966	3'-Hydroxy-4'-O-Methylglabridin
Gancao	MOL000497	licochalcone a
Gancao	MOL004974	3'-Methoxyglabridin
Gancao	MOL004978	2-[(3R)-8,8-dimethyl-3,4-dihydro-2H-pyrano[6,5-f]chromen-3-yl]-5-methoxyphenol
Gancao	MOL004980	Inlicoumarin A
Gancao	MOL004985	icos-5-enoic acid
Gancao	MOL004988	Kanzonol F
Gancao	MOL004989	6-prenylated eriodictyol
Gancao	MOL004990	7,2',4'-trihydroxy-5-methoxy-3-arylcoumarin
Gancao	MOL004991	7-Acetoxy-2-methylisoflavone
Gancao	MOL004993	8-prenylated eriodictyol
Gancao	MOL004996	gadelaidic acid
Gancao	MOL000500	Vestitol
Gancao	MOL000500	Gancaonin G
Gancao	MOL000500	Gancaonin H
Gancao	MOL000503	Licoagrocarpin
Gancao	MOL000507	Glyasperin M
Gancao	MOL000508	Glycyrrhiza flavonol A
Gancao	MOL000512	Licoagroisoflavone
Gancao	MOL000513	18α-hydroxyglycyrrhetic acid
Gancao	MOL000516	Odoratin
Gancao	MOL000517	Phaseol
Gancao	MOL000518	Xambioona
Gancao	MOL000520	dehydroglyasperin C
Gancao	MOL000098	quercetin

CHSGS, Chai Hu Shu Gan San; TCM, traditional Chinese medicine.

Table S2 The active components of LSJZSF

TCM	Mol ID	Molecule Name
Chishao	MOL001002	ellagic acid
Chishao	MOL001918	paeoniflorgenone
Chishao	MOL001921	Lactiflorin
Chishao	MOL001924	paeoniflorin
Chishao	MOL001925	paeoniflorin_qt
Chishao	MOL002714	baicalein
Chishao	MOL002776	Baicalin
Chishao	MOL000358	beta-sitosterol
Chishao	MOL000359	sitosterol
Chishao	MOL004355	Spinasterol
Chishao	MOL000449	Stigmasterol
Chishao	MOL000492	(+)-catechin
Chishao	MOL006990	(1S,2S,4R)-trans-2-hydroxy-1,8-cineole-B-D-glucopyranoside
Chishao	MOL006992	(2R,3R)-4-methoxy-distylin
Chishao	MOL006994	1-o-beta-d-glucopyranosyl-8-o-benzoylpaeonisuffrone_qt
Chishao	MOL006996	1-o-beta-d-glucopyranosylpaeonisuffrone_qt
Chishao	MOL006999	stigmast-7-en-3-ol
Chishao	MOL007003	benzoyl paeoniflorin
Chishao	MOL007004	Albiflorin
Chishao	MOL007005	Albiflorin_qt
Chishao	MOL007008	4-ethyl-paeoniflorin_qt
Chishao	MOL007012	4-o-methyl-paeoniflorin_qt
Chishao	MOL007014	8-debenzoylpaeonidanin
Chishao	MOL007016	Paeoniflorigenone
Chishao	MOL007018	9-ethyl-neo-paeoniaflorin A_qt
Chishao	MOL007022	evofolinB
Chishao	MOL007025	isobenzoylpaeoniflorin
Chishao	MOL002883	Ethyl oleate (NF)
Chishao	MOL005043	campest-5-en-3beta-ol
Zhebeimu	MOL001004	pelargonidin
Zhebeimu	MOL000358	beta-sitosterol
Zhebeimu	MOL004440	Peimisine
Zhebeimu	MOL004443	Zhebeiresinol
Zhebeimu	MOL004444	Ziebeimine
Zhebeimu	MOL004446	6-Methoxy-2-acetyl-3-methyl-1,4-naphthoquinone-8-O-beta-D-glucopyranoside
Zhebeimu	MOL004450	Chaksine
Nanshashen	MOL002883	Ethyl oleate (NF)
Nanshashen	MOL000358	beta-sitosterol
Nanshashen	MOL001494	Mandenol
Nanshashen	MOL003479	cycloartenol acetate
Nanshashen	MOL003485	Phthalic acid, isobutyl undecyl ester
Huangjing	MOL001792	DFV
Huangjing	MOL002714	baicalein
Huangjing	MOL002959	3'-Methoxydaidzein
Huangjing	MOL000358	beta-sitosterol
Huangjing	MOL000359	sitosterol
Huangjing	MOL003889	methylprotodioscin_qt
Huangjing	MOL004941	(2R)-7-hydroxy-2-(4-hydroxyphenyl)chroman-4-one
Huangjing	MOL000546	diosgenin
Huangjing	MOL006331	4',5'-Dihydroxyflavone
Huangjing	MOL009760	sibiricoside A_qt
Huangjing	MOL009763	(+)-Syringaresinol-O-beta-D-glucoside
Huangjing	MOL009766	zhonghualiaoine 1
Huangqin	MOL001689	acacetin
Huangqin	MOL000173	wogonin
Huangqin	MOL000228	(2R)-7-hydroxy-5-methoxy-2-phenylchroman-4-one
Huangqin	MOL002714	baicalein
Huangqin	MOL002908	5,8,2'-Trihydroxy-7-methoxyflavone
Huangqin	MOL002909	5,7,2',5-tetrahydroxy-8,6-dimethoxyflavone
Huangqin	MOL002910	Carthamidin
Huangqin	MOL002911	2,6,2',4'-tetrahydroxy-6'-methoxychaleone
Huangqin	MOL002913	Dihydrobaicalin_qt
Huangqin	MOL002914	Eriodyctiol (flavanone)
Huangqin	MOL002915	Salvigenin
Huangqin	MOL002917	5,2',6'-Trihydroxy-7,8-dimethoxyflavone
Huangqin	MOL002925	5,7,2',6'-Tetrahydroxyflavone
Huangqin	MOL002926	dihydrooroxilin A
Huangqin	MOL002927	Skullcapflavone II
Huangqin	MOL002928	oroxilin a
Huangqin	MOL002932	Panicolin
Huangqin	MOL002933	5,7,4'-Trihydroxy-8-methoxyflavone
Huangqin	MOL002934	NEOBAICALEIN
Huangqin	MOL002937	DIHYDROOROXYLIN
Huangqin	MOL000358	beta-sitosterol
Huangqin	MOL000359	sitosterol
Huangqin	MOL000525	Norwogonin
Huangqin	MOL000552	5,2'-Dihydroxy-6,7,8-trimethoxyflavone
Huangqin	MOL000073	ent-Epicatechin
Huangqin	MOL000449	Stigmasterol
Huangqin	MOL001458	coptisine
Huangqin	MOL001490	bis[(2S)-2-ethylhexyl] benzene-1,2-dicarboxylate
Huangqin	MOL001506	Supraene
Huangqin	MOL002879	Diop
Huangqin	MOL002897	epiberberine
Huangqin	MOL008206	Mososooflavone
Huangqin	MOL010415	11,13-Eicosadienoic acid, methyl ester
Huangqin	MOL012245	5,7,4'-trihydroxy-6-methoxyflavanone
Huangqin	MOL012246	5,7,4'-trihydroxy-8-methoxyflavanone
Huangqin	MOL012266	rivularin
Lianqiao	MOL000173	wogonin
Lianqiao	MOL003281	20(S)-dammar-24-ene-3β,20-diol-3-acetate
Lianqiao	MOL003283	(2R,3R,4S)-4-(4-hydroxy-3-methoxy-phenyl)-7-methoxy-2,3-dimethylol-tetralin-6-ol
Lianqiao	MOL003290	(3R,4R)-3,4-bis[(3,4-dimethoxyphenyl)methyl]oxolan-2-one
Lianqiao	MOL003295	(+)-pinoresinol monomethyl ether
Lianqiao	MOL003305	PHILLYRIN
Lianqiao	MOL003306	ACon1_001697
Lianqiao	MOL003308	(Con)-pinoresinol monomethyl ether-4-D-beta-glucoside_qt
Lianqiao	MOL003315	3beta-Acetyl-20,25-epoxydammarane-24alpha-ol
Lianqiao	MOL000211	Mairin
Lianqiao	MOL003322	FORSYTHINOL
Lianqiao	MOL003330	(-)-Phillygenin
Lianqiao	MOL003344	β-amyryn acetate
Lianqiao	MOL003347	hyperforin
Lianqiao	MOL003348	adhyperforin
Lianqiao	MOL003365	Lactucasterol
Lianqiao	MOL003370	Onjixanthone I
Lianqiao	MOL000358	beta-sitosterol
Lianqiao	MOL000422	kaempferol
Lianqiao	MOL000522	arctiin
Lianqiao	MOL000006	luteolin
Lianqiao	MOL000791	bicuculline
Lianqiao	MOL000098	quercetin
Yuxingcao	MOL003851	Isoramanone
Yuxingcao	MOL000422	kaempferol
Yuxingcao	MOL004345	1-methyl-2-nonacosyl-4-quinolone
Yuxingcao	MOL004350	Ruvoside_qt
Yuxingcao	MOL004351	C09747
Yuxingcao	MOL004355	Spinasterol
Yuxingcao	MOL000098	quercetin
Zhike	MOL013381	Marmin
Zhike	MOL002341	Hesperetin
Zhike	MOL000358	beta-sitosterol
Zhike	MOL004328	naringenin
Zhike	MOL005828	nobiletin
Gancao	MOL001484	Inermine
Gancao	MOL001792	DFV
Gancao	MOL000211	Mairin
Gancao	MOL002311	Glycyrol
Gancao	MOL000239	Jaranol
Gancao	MOL002565	Medicarpin
Gancao	MOL000354	isorhamnetin
Gancao	MOL000359	sitosterol
Gancao	MOL003656	Lupiwighteone
Gancao	MOL003896	7-Methoxy-2-methyl isoflavone
Gancao	MOL000392	formononetin
Gancao	MOL000417	Calycosin
Gancao	MOL000422	kaempferol
Gancao	MOL004328	naringenin
Gancao	MOL004805	(2S)-2-[4-hydroxy-3-(3-methylbut-2-enyl)phenyl]-8,8-dimethyl-2,3-dihydropyranol[2,3-f]chromen-4-one
Gancao	MOL004806	euchrenone
Gancao	MOL004807	glyasperin B
Gancao	MOL004810	glyasperin F
Gancao	MOL004811	Glyasperin C
Gancao	MOL004814	Isotrifolol
Gancao	MOL004815	(E)-1-(2,4-dihydroxyphenyl)-3-(2,2-dimethylchromen-6-yl)prop-2-en-1-one
Gancao	MOL004820	kanzonols W
Gancao	MOL004824	(2S)-6-(2,4-dihydroxyphenyl)-2-(2-hydroxypropan-2-yl)-4-methoxy-2,3-dihydrofuro[3,2-g]chromen-7-one
Gancao	MOL004827	Semilicoisoflavone B
Gancao	MOL004828	Glepidotin A
Gancao	MOL004829	Glepidotin B
Gancao	MOL004833	Phaseolinisoflavan
Gancao	MOL004835	Glypallichalcone
Gancao	MOL004838	8-(6-hydroxy-2-benzofuranyl)-2,2-dimethyl-5-chromenol
Gancao	MOL004841	Licochalcone B
Gancao	MOL004848	licoachalcone G
Gancao	MOL004849	3-(2,4-dihydroxyphenyl)-8-(1,1-dimethylprop-2-enyl)-7-hydroxy-5-methoxy-coumarin
Gancao	MOL004855	Licoricone
Gancao	MOL004856	Gancaonin A
Gancao	MOL004857	Gancaonin B
Gancao	MOL004860	licorice glycoside E
Gancao	MOL004863	3-(3,4-dihydroxyphenyl)-5,7-dihydroxy-8-(3-methylbut-2-enyl)chromone
Gancao	MOL004864	5,7-dihydroxy-3-(4-methoxyphenyl)-8-(3-methylbut-2-enyl)chromone
Gancao	MOL004866	2-(3,4-dihydroxyphenyl)-5,7-dihydroxy-6-(3-methylbut-2-enyl)chromone
Gancao	MOL004879	Glycyrin
Gancao	MOL004882	Licocoumarone
Gancao	MOL004883	Licoisoflavone
Gancao	MOL004884	Licoisoflavone B
Gancao	MOL004885	licoisoflavanone
Gancao	MOL004891	shinpterocarpin
Gancao	MOL004898	(E)-3-[3,4-dihydroxy-5-(3-methylbut-2-enyl)phenyl]-1-(2,4-dihydroxyphenyl)prop-2-en-1-one
Gancao	MOL004903	liquiritin
Gancao	MOL004904	licopyranocoumarin
Gancao	MOL004905	3,22-Dihydroxy-11-oxo-delta(12)-oleanene-27-alpha-methoxycarbonyl-29-oxic acid
Gancao	MOL004907	Glyzaglabrin
Gancao	MOL004908	Glabridin
Gancao	MOL004910	Glabranin
Gancao	MOL004911	Glabrene
Gancao	MOL004912	Glabrone
Gancao	MOL004913	1,3-dihydroxy-9-methoxy-6-benzofurano[3,2-c]chromenone
Gancao	MOL004914	1,3-dihydroxy-8,9-dimethoxy-6-benzofurano[3,2-c]chromenone
Gancao	MOL004915	Eurycarpin A
Gancao	MOL004917	glycyroside
Gancao	MOL004924	(-)-Medicocarpin
Gancao	MOL004935	Sigmoidin-B
Gancao	MOL004941	(2R)-7-hydroxy-2-(4-hydroxyphenyl)chroman-4-one
Gancao	MOL004945	(2S)-7-hydroxy-2-(4-hydroxyphenyl)-8-(3-methylbut-2-enyl)chroman-4-one
Gancao	MOL004948	Isoglycyrol
Gancao	MOL004949	Isolicoflavonol
Gancao	MOL004957	HMO
Gancao	MOL004959	1-Methoxyphaseollidin
Gancao	MOL004961	Quercetin der.
Gancao	MOL004966	3'-Hydroxy-4'-O-Methylglabridin
Gancao	MOL00497	licoachalcone a
Gancao	MOL004974	3'-Methoxyglabridin
Gancao	MOL004978	2-[[3(R)-8,8-dimethyl-3,4-dihydro-2H-pyran[6,5-f]chromen-3-yl]]-5-methoxyphenol
Gancao	MOL004980	Inflacoumarin A
Gancao	MOL004985	icos-5-enoic acid
Gancao	MOL004988	Kanzonol F
Gancao	MOL004989	6-prenylated eriodictyol
Gancao	MOL004990	7,2',4'-trihydroxy-5-methoxy-3-arylcoumarin
Gancao	MOL004991	7-Acetoxy-2-methylisoflavone
Gancao	MOL004993	8-prenylated eriodictyol
Gancao	MOL004996	gadelaidic acid
Gancao	MOL000500	Vestitol
Gancao	MOL005000	Gancaonin G
Gancao	MOL005001	Gancaonin H
Gancao	MOL005003	Licoagrocarpin
Gancao	MOL005007	Glyasperins M
Gancao	MOL005008	Glycyrrhiza flavonol A
Gancao	MOL005012	Licoagroisoflavone
Gancao	MOL005013	18α-hydroxyglycyrrhetic acid
Gancao	MOL005016	Odoratin
Gancao	MOL005017	Phaseol
Gancao	MOL005018	Xambioona
Gancao	MOL005020	dehydroglyasperins C
Gancao	MOL000098	quercetin

LSJZSF, Li Shi Jian Zhi Shu Fang; TCM, traditional Chinese medicine.

Table S3 The active components of SNSHSJS

TCM	Mol ID	Molecule name
Chaihu	MOL001645	Linoleyl acetate
Chaihu	MOL002776	Baicalin
Chaihu	MOL000449	Stigmasterol
Chaihu	MOL000354	isorhamnetin
Chaihu	MOL000422	kaempferol
Chaihu	MOL004598	3,5,6,7-tetramethoxy-2-(3,4,5-trimethoxyphenyl)chromone
Chaihu	MOL004609	Areapillin
Chaihu	MOL013187	Cubebin
Chaihu	MOL004624	Longikaurin A
Chaihu	MOL004628	Octalupine
Chaihu	MOL004644	Sainfuran
Chaihu	MOL004648	Troxeutin
Chaihu	MOL004653	(+)-Anomalin
Chaihu	MOL004702	saikosaponin c_qt
Chaihu	MOL004718	α -spinasterol
Chaihu	MOL000490	petunidin
Chaihu	MOL000098	quercetin
Baishao	MOL001910	11alpha,12alpha-epoxy-3beta-23-dihydroxy-30-norolean-20-en-28,12beta-olide
Baishao	MOL001918	paeoniflorgenone
Baishao	MOL001919	(3S,5R,8R,9R,10S,14S)-3,17-dihydroxy-4,4,8,10,14-pentamethyl-2,3,5,6,7,9-hexahydro-1H-cyclopenta[a]phenanthrene-15,16-dione
Baishao	MOL001921	Lactiflorin
Baishao	MOL001924	paeoniflorin
Baishao	MOL001925	paeoniflorin_qt
Baishao	MOL001928	albiflorin_qt
Baishao	MOL001930	benzoyl paeoniflorin
Baishao	MOL000211	Mairin
Baishao	MOL000358	beta-sitosterol
Baishao	MOL000359	sitosterol
Baishao	MOL000422	kaempferol
Baishao	MOL000492	(+)-catechin
Jiangcan	MOL000098	quercetin
Jiangcan	MOL000422	kaempferol
Jiangcan	MOL000359	sitosterol
Jianghuang	MOL000449	Stigmasterol
Jianghuang	MOL000493	campesterol
Jianghuang	MOL000953	CLR
Zhike	MOL013381	Marmin
Zhike	MOL002341	Hesperetin
Zhike	MOL000358	beta-sitosterol
Zhike	MOL004328	naringenin
Zhike	MOL005828	nobiletin
Gancao	MOL001484	Inermine
Gancao	MOL001792	DFV
Gancao	MOL000211	Mairin
Gancao	MOL002311	Glycyrol
Gancao	MOL000239	Jaranol
Gancao	MOL002565	Medicarpin
Gancao	MOL000354	isorhamnetin
Gancao	MOL000359	sitosterol
Gancao	MOL003656	Lupiwighteone
Gancao	MOL003896	7-Methoxy-2-methyl isoflavone
Gancao	MOL000392	formononetin
Gancao	MOL000417	Calycosin
Gancao	MOL000422	kaempferol
Gancao	MOL004328	naringenin
Gancao	MOL004805	(2S)-2-[4-hydroxy-3-(3-methylbut-2-enyl)phenyl]-8,8-dimethyl-2,3-dihydroprano[2,3-f]chromen-4-one
Gancao	MOL004806	euchrenone
Gancao	MOL004808	glyasperin B
Gancao	MOL004810	glyasperin F
Gancao	MOL004811	Glyasperin C
Gancao	MOL004814	Isotrifoliol
Gancao	MOL004815	(E)-1-(2,4-dihydroxyphenyl)-3-(2,2-dimethylchromen-6-yl)prop-2-en-1-one
Gancao	MOL004820	kanzonols W
Gancao	MOL004824	(2S)-6-(2,4-dihydroxyphenyl)-2-(2-hydroxypropan-2-yl)-4-methoxy-2,3-dihydrofuro[3,2-g]chromen-7-one
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Gancao	MOL005017	Phaseol
Gancao	MOL005018	Xambioona
Gancao	MOL005020	dehydroglyasperin C
Gancao	MOL000098	quercetin

SNSHSJS, Si Ni San He Sheng Jiang San; TCM, traditional Chinese medicine.

Table S4 Top 5 hub genes with MCC scores

Genes	MCC
<i>TNF</i>	85920
<i>ICAM-1</i>	85920
<i>VEGFA</i>	85920
<i>CRP</i>	85800
<i>IFN-γ</i>	85680

MCC, Maximal Clique Centrality; *TNF*, tumor necrosis factor; *ICAM-1*, intercellular adhesion molecule 1; *VEGFA*, vascular endothelial growth factor A; *CRP*, C-reactive protein; *IFN- γ* , interferon gamma.