

Supplementary Table S1. Chemical information database for the components of DS and HH

Source	Compound name	Molecular formula
HH	(-)-17-Hydroxy-16beta-kauran-19-oicacid	C ₂₀ H ₃₂ O ₃
HH	(-)-α-cedrene	C ₁₅ H ₂₄
HH	(3E,5Z)-1,3,5-tridecatrien-7,9,11-triyne	C ₁₃ H ₁₀
HH	(E)-1,3-tridecadiene-5,7,9,11-tetrayne	C ₁₃ H ₈
HH	(E)-2-hexenal	C ₆ H ₁₀ O
HH	(E)-3-Tridecene-5,7,9,11-tetrayne-1,2-diol	C ₁₃ H ₁₀ O ₂
HH	(E,E)-1,3,5-tridecatriene-7,9,11-triyne	C ₁₃ H ₁₀
HH	(E,E)-2,4-decadial	C ₁₀ H ₁₆ O
HH	(E,E,E)-1,3,5,11-tridecatetraene-7,9-diyne	C ₁₃ H ₁₂
HH	(Z)-1,11-tridecadiene-3,5,7,9-tetrayne	C ₁₃ H ₈
HH	(Z)-1,3-tridecadiene-5,7,9,11-tetrayne	C ₁₃ H ₈
HH	(Z,E)-1,3,11-tridecatriene-5,7,9-triyne	C ₁₃ H ₁₀
HH	(Z,Z)-1,3,11-tridecatriene-5,7,9-triyne	C ₁₃ H ₁₀
HH	(Z,Z)-1,8,11-heptadecatriene	C ₁₇ H ₃₀
HH	(Z,Z,Z)-1,8,11,14-heptadecatetraene	C ₁₇ H ₂₈
HH	1,11-tridecadiene-3,5,7,9-tetrayne	C ₁₃ H ₈
HH	1,2,3-trimethoxy-5-methylbenzene	C ₁₀ H ₁₄ O ₃
DS	1,2-dihydrotanshinquinone	C ₁₈ H ₁₄ O ₃
HH	1,3,11-tridecatrien-5,7,9-triyne	C ₁₃ H ₁₀
DS	1,5-dihydroxy-3-methylanthraquinone	C ₁₅ H ₁₀ O ₄
DS	12-hydroxy-6,7-secoabieta-8,11,13-triene-6,7-dial	C ₂₀ H ₂₈ O ₃
HH	1-heptadecene	C ₁₇ H ₃₄
HH	1-hexadecene	C ₁₆ H ₃₂
DS	1-hydroxytaxinine A	C ₂₆ H ₃₆ O ₉
DS	1-ketoisocryptotanshinone	C ₁₉ H ₁₈ O ₄
HH	1-pentadecene	C ₁₅ H ₃₀
HH	1-pentene-3-ol	C ₅ H ₁₀ O
HH	1-tetradecene	C ₁₄ H ₂₈
HH	1-tridecene-3,5,7,9,11-pentayne	C ₁₃ H ₆
DS	2,3,19-trihydroxyurs-12-en-28-oic acid	C ₃₀ H ₄₈ O ₅
HH	20-hexadecanoylingenol	C ₃₆ H ₅₈ O ₆
HH	2-hexanol	C ₆ H ₁₄ O
DS	2-isopropyl-8-methylphenanthrene-3,4-dione	C ₁₈ H ₁₆ O ₂
HH	2-methylbutyric acid	C ₅ H ₁₀ O ₂
HH	3,11-Tridecadiene-5,7,9-triyne-1,2-diol	C ₁₃ H ₁₂ O ₂
HH	3,4-dihydroxyrottlerin	C ₃₀ H ₂₈ O ₁₀
DS	3α-hydroxytanshinone IIA	C ₁₉ H ₁₈ O ₄
DS	3β-hydroxytanshinone IIA	C ₁₉ H ₁₈ O ₄
HH	3-hexanol	C ₆ H ₁₄ O
HH	3-methylbutyric acid	C ₅ H ₁₀ O ₂
DS	3-O-acetyloleanolic acid	C ₃₂ H ₅₀ O ₄

DS	3-β-hydroxymethylenetanshiquinone	C ₁₈ H ₁₄ O ₄
DS	4-methylsalicylaldehyde	C ₈ H ₈ O ₂
HH	4-terpineol	C ₁₀ H ₁₈ O
HH	5,6,7,4'-tetrahydroxyflavanone 6,7-di-O-b-D-glucoside	C ₂₇ H ₃₂ O ₁₆
HH	5,6-dehydrosugiol	C ₂₀ H ₂₆ O ₂
HH	5,7-dihydroxy-4'-methoxyflavone-7-O-b-D-apiofuranosyl-(1-6)-O-b-D-glucoside	C ₂₇ H ₃₀ O ₁₄
product	5-hydroxymethylfurfural	C ₆ H ₆ O ₃
DS	6,12-dihydroxyabieta-5,8,11,13-tetraen-7-one	C ₂₀ H ₂₆ O ₃
HH	6,8-nonacosanediol	C ₂₉ H ₆₀ O ₂
HH	6-hydroxykaempferol	C ₁₅ H ₁₀ O ₇
HH	6-hydroxykaempferol-3,6,7-tri-O-glucoside	C ₃₃ H ₄₀ O ₂₂
HH	6-hydroxykaempferol-3,6-di-O-glucoside	C ₂₇ H ₃₀ O ₁₇
HH	6-hydroxykaempferol-3,6-di-O-glucoside-7-O-glucuronide	C ₃₃ H ₃₈ O ₂₃
HH	6-hydroxykaempferol-3-O-glucoside	C ₂₁ H ₂₀ O ₁₂
HH	6-hydroxykaempferol-3-O-rutinoside-6-O-glucoside	C ₃₃ H ₄₀ O ₂₁
HH	6-hydroxykaempferol-6,7-di-O-glucoside	C ₂₇ H ₃₀ O ₁₇
HH	6-hydroxykaempferol-7-O-glucoside	C ₂₁ H ₂₀ O ₁₂
DS	6-hydroxymethylumazin	C ₇ H ₆ N ₄ O ₃
DS	6α-hydroxysugiol	C ₂₀ H ₂₈ O ₃
DS	7-dehydroabietanone	C ₂₀ H ₂₈ O
DS	8β-hydroxy-9(11),13-abietadien-12-one	C ₂₀ H ₃₀ O ₂
HH	adenosine	C ₁₀ H ₁₃ N ₅ O ₄
HH	alexandrin	C ₃₅ H ₆₀ O ₆
HH	alpha-onocerin	C ₃₀ H ₅₀ O ₂
HH	anhydrosafflor yellow B	C ₄₈ H ₅₂ O ₂₆
HH	apigenin	C ₁₅ H ₁₀ O ₅
HH	arabinose	C ₅ H ₁₀ O ₅
HH	arachidic acid	C ₂₀ H ₄₀ O ₂
DS	baicalin	C ₂₁ H ₁₈ O ₁₁
HH	benzothiazole	C ₇ H ₅ NS
DS	caffeic acid	C ₉ H ₈ O ₄
HH	caffeic acid	C ₉ H ₈ O ₄
HH	carthamin	C ₄₃ H ₄₂ O ₂₂
HH	carthamone	C ₂₁ H ₂₀ O ₁₁
HH	cartorimine	C ₁₅ H ₁₄ O ₆
HH	cartormin	C ₂₇ H ₂₉ NO ₁₃
HH	carvacrol	C ₁₀ H ₁₄ O
HH	caryophyllene	C ₁₅ H ₂₄
HH	caryophyllene epoxide	C ₁₅ H ₂₄ O
HH	chlorogenic acid	C ₁₆ H ₁₈ O ₉
HH	cholesterol	C ₂₇ H ₄₆ O
HH	cis-9-octadecenoic acid	C ₁₈ H ₃₄ O ₂

HH	clinodiside A	C ₄₈ H ₇₈ O ₁₉
HH	cnidilin	C ₁₇ H ₁₆ O ₅
HH	copaene	C ₁₅ H ₂₄
DS	corosolicacid	C ₃₀ H ₄₈ O ₄
DS	cryptoacetalide	C ₁₈ H ₂₂ O ₃
DS	cryptotanshinone	C ₁₉ H ₂₀ O ₃
DS	cryptoxanthin	C ₄₀ H ₅₆ O
HH	D-(+)-Galactose	C ₆ H ₁₂ O ₆
DS	danshenol A	C ₂₁ H ₂₀ O ₄
DS	danshenol B	C ₂₂ H ₂₆ O ₄
DS	danshenol C	C ₂₁ H ₂₀ O ₄
DS	danshenspiroketallactone	C ₁₇ H ₁₆ O ₃
DS	danshensu	C ₉ H ₁₀ O ₅
DS	danshensuan B	C ₃₆ H ₃₀ O ₁₆
DS	danshenxinkun A	C ₁₈ H ₁₆ O ₄
DS	danshenxinkun B	C ₁₈ H ₁₆ O ₃
DS	danshenxinkun C	C ₁₆ H ₁₂ O ₃
DS	danshenxinkun D	C ₂₁ H ₂₀ O ₄
DS	daphneolone	C ₁₇ H ₁₈ O ₃
DS	daucosterol	C ₃₅ H ₆₀ O ₆
HH	daucosterol	C ₃₅ H ₆₀ O ₆
DS	dauricine	C ₃₈ H ₄₄ N ₂ O ₆
HH	decanal	C ₁₀ H ₂₀ O
DS	dehydromiltirone	C ₁₉ H ₂₀ O ₂
DS	dehydromorroniaglycone	C ₁₁ H ₁₄ O ₅
HH	dehydroshikimic acid	C ₇ H ₈ O ₅
DS	dehydrotremetone	C ₁₃ H ₁₂ O ₂
DS	deoxyneocryptotanshinone	C ₁₅ H ₁₃ N ₃ O
HH	dihydroactinidiolide	C ₁₁ H ₁₆ O ₂
DS	dihydroisotanshinone I	C ₁₈ H ₁₄ O ₃
DS	dihydroisotanshinone II	C ₁₈ H ₁₄ O ₃
DS	dihydrokaranone	C ₁₅ H ₂₂ O
DS	dihydroneotanshinlactone	C ₁₇ H ₁₄ O ₃
DS	dihydronortanshinone	C ₁₇ H ₁₄ O ₄
DS	dihydrotanshinone I	C ₁₈ H ₁₄ O ₃
DS	dihydrovalepotriate	C ₂₃ H ₃₄ O ₈
DS	dimethylthiospermate	C ₂₉ H ₂₆ O ₁₂
HH	dipalmitin	C ₃₅ H ₆₈ O ₅
HH	D-mannose	C ₆ H ₁₂ O ₆
HH	dopa	C ₉ H ₁₁ NO ₄
DS	eleutheroside A	C ₃₅ H ₆₀ O ₆
DS	epi-cryptoacetalide	C ₁₈ H ₂₂ O ₃
DS	epi-danshenspiroketallactone	C ₁₇ H ₁₆ O ₃
DS	epi-danshenspiroketallactone A	C ₂₀ H ₂₀ O ₅

HH	eriodictyol	$C_{15}H_{12}O_6$
HH	ethylacetate	$C_4H_8O_2$
HH	ethylbenzene	C_8H_{10}
DS	ferruginol	$C_{20}H_{30}O$
DS	ferulic acid	$C_{10}H_{10}O_4$
DS	gamma-sitosterol	$C_{29}H_{50}O$
HH	gamma-sitosterol	$C_{29}H_{50}O$
HH	guanosine	$C_{10}H_{13}N_5O_5$
DS	heteratisine	$C_{22}H_{33}NO_5$
HH	humulene	$C_{15}H_{24}$
HH	hydroxysafflor yellow A	$C_{27}H_{32}O_{16}$
DS	hydroxytanshinone IIA	$C_{19}H_{18}O_4$
DS	isocryptotanshinone	$C_{19}H_{20}O_3$
DS	isocucurbitacin D	$C_{30}H_{44}O_7$
DS	isoferulic acid	$C_{10}H_{10}O_4$
DS	isoimperatorin	$C_{16}H_{14}O_4$
DS	isotanshinone I	$C_{18}H_{12}O_3$
DS	isotanshinone IIA	$C_{19}H_{18}O_3$
DS	isotanshinone IIB	$C_{19}H_{18}O_4$
DS	isotenulin	$C_{17}H_{22}O_5$
DS	isototanshinone	$C_{17}H_{12}O_3$
HH	kaempferol	$C_{15}H_{10}O_6$
HH	kaempferol-3-O-glucoside	$C_{21}H_{20}O_{11}$
HH	kaempferol-3-O-glucoside-7-O-glucuronide	$C_{27}H_{28}O_{17}$
HH	kaempferol-3-O-rutinoside	$C_{27}H_{30}O_{15}$
HH	kaempferol-3-O-sophorose	$C_{27}H_{30}O_{16}$
HH	L-(+)-arabinose	$C_5H_{10}O_5$
HH	lauric aldehyde	$C_{12}H_{24}O$
HH	linoleic acid	$C_{18}H_{32}O_2$
HH	linoleylacetate	$C_{20}H_{36}O_2$
HH	linolic acid	$C_{18}H_{32}O_2$
DS	lithospermic acid dimethyl ester	$C_{29}H_{26}O_{12}$
DS	lithospermic acid monomethyl ester	$C_{28}H_{24}O_{12}$
DS	lithospermate B	$C_{36}H_{30}MgO_{16}$
DS	lithospermic acid	$C_{27}H_{22}O_{12}$
DS	lithospermic acid B	$C_{36}H_{30}O_{16}$
HH	luteolin	$C_{15}H_{10}O_6$
HH	lysine	$C_6H_{14}N_2O_2$
HH	methylcinnamate	$C_{10}H_{10}O_2$
DS	methyldihydronortanshinonate	$C_{20}H_{20}O_5$
DS	methylenetanshinquinone	$C_{18}H_{14}O_3$
DS	methylrosmarinate	$C_{19}H_{18}O_8$
DS	methyltanshinonate	$C_{20}H_{18}O_5$
DS	methyltanshinquinon	$C_{18}H_{16}O_3$

DS	miltiodiol	$C_{19}H_{22}O_3$
DS	miltionone I	$C_{19}H_{20}O_4$
DS	miltionone II	$C_{19}H_{20}O_4$
DS	miltipolone	$C_{19}H_{24}O_3$
DS	miltirone	$C_{19}H_{22}O_2$
DS	mimengoside A	$C_{54}H_{88}O_{21}$
DS	monomethyl lithospermate B	$C_{18}H_{22}O_5$
DS	mono-O-methylwightin	$C_{19}H_{18}O_7$
HH	myricetin	$C_{15}H_{10}O_8$
HH	myristic acid	$C_{14}H_{28}O_2$
HH	myristicin	$C_{11}H_{12}O_3$
HH	neocarthamin	$C_{21}H_{22}O_{11}$
HH	neocembrene	$C_{20}H_{32}$
DS	neocryptotanshinone II	$C_{17}H_{18}O_3$
DS	neosalvianen	$C_{21}H_{21}NO_2$
DS	neotanshinone B	$C_{18}H_{16}O_3$
DS	neotanshinone C	$C_{16}H_{12}O_3$
DS	neotigogenin	$C_{27}H_{44}O_3$
HH	nonacosane	$C_{29}H_{60}$
DS	normiltioane	$C_{18}H_{26}O_2$
DS	nortanshinone	$C_{17}H_{14}O_5$
DS	nortrachelogenin	$C_{20}H_{22}O_7$
DS	oleanolic acid	$C_{30}H_{48}O_3$
DS	oleoyl danshenxinkun A	$C_{36}H_{48}O_5$
DS	oleoyl neocryptotanshinone	$C_{37}H_{54}O_5$
DS	O-methyltaxodine	$C_{20}H_{29}NO_3$
HH	onjixanthone II	$C_{15}H_{12}O_7$
DS	paramiltioic acid	$C_{19}H_{24}O_5$
DS	<i>p</i> -coumaric acid	$C_9H_8O_3$
HH	phenylacetaldehyde	C_8H_8O
DS	phenylalanine	$C_9H_{11}NO_2$
HH	precarthamin	$C_{44}H_{46}O_{24}$
DS	prolithospermic acid	$C_{18}H_{14}O_8$
DS	protocatechuic acid	$C_7H_6O_4$
DS	protocatechuic acid-3-glucoside	$C_{13}H_{16}O_9$
DS	protocatechuic aldehyde	$C_7H_6O_3$
DS	przewalskin	$C_{18}H_{24}O_2$
DS	przewanoic acid B	$C_{29}H_{42}O_4$
DS	przewaquinone A	$C_{19}H_{18}O_4$
DS	przewaquinone B	$C_{18}H_{12}O_4$
DS	przewaquinone C	$C_{18}H_{16}O_4$
HH	pyrocatechol	$C_6H_6O_2$
HH	quercetin	$C_{15}H_{10}O_7$
HH	quercetin-3,7-di-O-glucoside	$C_{27}H_{30}O_{17}$

HH	quercetin-3-O-glucoside	$C_{21}H_{20}O_{12}$
HH	quercetin-3-O-rhamnoside-7-O-glucuronide	$C_{27}H_{28}O_{17}$
HH	quercetin-7-O-glucoside	$C_{21}H_{20}O_{12}$
HH	rhamnose	$C_6H_{12}O_5$
DS	rosmarinic acid	$C_{18}H_{16}O_8$
DS	rosmarinine	$C_{18}H_{27}NO_6$
HH	rutin	$C_{27}H_{30}O_{16}$
HH	safflomin A	$C_{27}H_{32}O_{16}$
HH	safflomin C	$C_{30}H_{30}O_{14}$
HH	safflor yellow A	$C_{27}H_{30}O_{15}$
HH	safflor yellow B	$C_{48}H_{54}O_{27}$
HH	safflower yellow	$C_{43}H_{42}O_{22}$
HH	safranal	$C_{10}H_{14}O$
HH	sagittariol	$C_{19}H_{32}O_2$
DS	salonitenolide	$C_{15}H_{20}O_4$
DS	salviadione	$C_{19}H_{19}NO_2$
DS	salvianen	$C_{21}H_{21}NO_2$
DS	salvianic acid A	$C_9H_{10}O_5$
DS	salvianic acid B	$C_{36}H_{30}O_{16}$
DS	salvianic acid C	$C_{18}H_{18}O_9$
DS	salvianolic acid A	$C_{26}H_{22}O_{10}$
DS	salvianolic acid B	$C_{36}H_{30}O_{16}$
DS	salvianolic acid C	$C_{26}H_{20}O_{10}$
DS	salvianolic acid D	$C_{20}H_{18}O_{10}$
DS	salvianolic acid E	$C_{36}H_{30}O_{16}$
DS	salvianolic acid F	$C_{17}H_{14}O_6$
DS	salvianolic acid G	$C_{18}H_{12}O_7$
DS	salvianolic acid I	$C_{27}H_{22}O_{12}$
DS	salvianolic acid J	$C_{27}H_{22}O_{12}$
DS	salvianolic acid N	$C_{26}H_{22}O_{10}$
DS	salvigenin	$C_{18}H_{16}O_6$
DS	salvilenone	$C_{20}H_{20}O_2$
DS	salvinal	$C_{20}H_{20}O_6$
DS	salvinone	$C_{18}H_{20}O_2$
DS	salviol	$C_{20}H_{30}O_2$
DS	salviolone	$C_{18}H_{20}O_2$
DS	samaderin A	$C_{18}H_{18}O_6$
HH	scutellarin	$C_{21}H_{18}O_{12}$
DS	sodium danshensu	$C_9H_9NaO_5$
HH	stearin	$C_{57}H_{110}O_6$
DS	stigmasterol	$C_{29}H_{48}O$
HH	stigmasterol	$C_{29}H_{48}O$
DS	succinic acid	$C_4H_6O_4$
DS	sugiol	$C_{20}H_{28}O_2$

DS	tanshinaldehyde	C ₁₉ H ₁₈ O ₄
DS	tanshinaldehyde II	C ₁₉ H ₁₆ O ₄
DS	tanshindiol A	C ₁₈ H ₁₆ O ₅
DS	tanshindiol A	C ₁₈ H ₁₆ O ₅
DS	tanshindiol B	C ₁₈ H ₁₆ O ₅
DS	tanshindiol C	C ₁₈ H ₁₆ O ₅
DS	tanshinketolactone	C ₁₈ H ₁₄ O ₄
DS	tanshinlactone	C ₁₇ H ₁₂ O ₃
DS	tanshinol A	C ₁₈ H ₁₂ O ₄
DS	tanshinol B	C ₁₈ H ₁₆ O ₄
DS	tanshinone I	C ₁₈ H ₁₂ O ₃
DS	tanshinone IIA	C ₁₉ H ₁₈ O ₃
DS	tanshinone IIB	C ₁₉ H ₁₈ O ₄
DS	tanshinone VI	C ₁₈ H ₁₆ O ₄
DS	tanshiquinone A	C ₁₈ H ₁₆ O ₄
DS	tanshiquinone B	C ₁₈ H ₁₆ O ₃
DS	tanshiquinone C	C ₁₆ H ₁₂ O ₃
DS	taraxanthin	C ₄₀ H ₅₆ O ₃
DS	tetrahydrotanshione	C ₁₈ H ₁₆ O ₃
DS	tigogenin	C ₂₇ H ₄₄ O ₃
HH	tinctormine	C ₂₁ H ₂₀ NO ₉
HH	tracheloside	C ₂₇ H ₃₄ O ₁₂
HH	trans-9-octadecenoic acid	C ₁₈ H ₃₄ O ₂
HH	uridine	C ₉ H ₁₂ N ₂ O ₆
DS	ursolic acid	C ₃₀ H ₄₈ O ₃
HH	verbenone	C ₁₀ H ₁₄ O
HH	xylene	C ₈ H ₁₀
HH	xylose	C ₅ H ₁₀ O ₅
HH	α-D-glucose	C ₆ H ₁₂ O ₆
HH	β-caryophyllene	C ₁₅ H ₂₄
HH	β-D-glucose	C ₆ H ₁₂ O ₆
HH	β-farnesene	C ₁₅ H ₂₄
HH	β-ionone	C ₁₃ H ₂₀ O
HH	β-sitosterol	C ₂₉ H ₅₀ O
