

Table S2. Active ingredients of Dayuanxiaodu (DYXX) herbal medicine.

ID	Compound	OB (%)	DL
MOL000483	(Z)-3-(4-hydroxy-3-methoxy-phenyl)-N-[2-(4-hydroxyphenyl)ethyl]acrylamide	118.35	0.26
MOL000631	Coumaroyltyramine	112.9	0.2
MOL007132	(2R)-3-(3,4-dihydroxyphenyl)-2-[(Z)-3-(3,4-dihydroxyphenyl)acryloyl]oxy-propionic acid	109.38	0.35
MOL002934	Neobaicalein	104.34	0.44
MOL003330	(-)-Phillygenin	95.04	0.57
MOL002311	Glycyrol	90.78	0.67
MOL013098	[(9R)-8,8-dimethyl-2-oxo-9,10-dihydropyrano[6,5-h]chromen-9-yl] (Z)-2-methylbut-2-enoate	87.48	0.37
MOL012922	l-SPD	87.35	0.54
MOL003306	ACon1_001697	85.12	0.57
MOL007747	Chloranoside a qt	84.11	0.23
MOL003322	Forsythinol	81.25	0.57
MOL000546	Diosgenin	80.88	0.81
MOL007742	Istanbulin-A	80.1	0.2
MOL004644	Sainfuran	79.91	0.23
MOL007207	Machiline	79.64	0.24
MOL003370	Onjixanthone I	79.16	0.3
MOL005017	Phaseol	78.77	0.58
MOL004841	Licochalcone B	76.76	0.19
MOL002932	Panicolin	76.26	0.29
MOL005890	Pachypodol	75.06	0.4
MOL012246	5,7,4'-trihydroxy-8-methoxyflavanone	74.24	0.26
MOL012583	(2R,3R,4S)-2-(3,4-dihydroxyphenyl)-4-(2,4,6-trihydroxyphenyl)chroman-3,5,7-triol	72.41	0.64
MOL013101	Rutarin qt	70.1	0.2
MOL000791	Bicuculline	69.67	0.88
MOL002927	Skullcapflavone II	69.51	0.44
MOL007206	Armepavine	69.31	0.29
MOL002911	2,6,2',4'-tetrahydroxy-6'-methoxychaleone	69.04	0.22
MOL000433	FA	68.96	0.71
MOL000074	(4E,6E)-1,7-bis(4-hydroxyphenyl)hepta-4,6-dien-3-one	67.92	0.24
MOL000004	Procyanidin B1	67.87	0.66
MOL006405	(1S)-1-(4-hydroxybenzyl)-2-methyl-3,4-dihydro-1H-isoquinoline-6,7-diol	67.14	0.23
MOL003410	Ziziphin qt	66.95	0.62
MOL003283	(2R,3R,4S)-4-(4-hydroxy-3-methoxy-phenyl)-7-methoxy-2,3-dimethylol-tetralin-6-ol	66.51	0.39
MOL002937	Dihydrooroxylin	66.06	0.23
MOL004903	Liquiritin	65.69	0.74
MOL012577	(2R,3R,10S)-2,10-bis(3,4-dihydroxyphenyl)-3,5-dihydroxy-3,4,9,10-tetrahydro-2H-pyrano[6,5-h]chromen-8-one	65.26	0.93
MOL013087	Peucedanocoumarin II	63.48	0.53
MOL000569	Digallate	61.85	0.26

MOL003308	(+)-pinoresinol monomethyl ether-4-D-beta-glucoside Qt	61.2	0.57
MOL004489	Anemarsaponin F Qt	60.06	0.79
MOL013093	Rubricauloside	58.36	0.71
MOL013095	Sporidesmin	58.31	0.76
MOL012579	(4R,8R,9R)-4,8-bis(3,4-dihydroxyphenyl)-5,9-dihydroxy-4,8,9,10-tetrahydro-3H-pyrano[6,5-h]chromen-2-one	58.16	0.93
MOL001677	asperglaucide	58.02	0.52
MOL010857	Sterigmato-cystin	57.16	0.68
MOL013187	Cubebin	57.13	0.64
MOL004792	nodakenin	57.12	0.69
MOL000211	Mairin	55.38	0.78
MOL000228	(2R)-7-hydroxy-5-methoxy-2-phenylchroman-4-one	55.23	0.2
MOL006821	(-)-epigallocatechin-3-gallate	55.09	0.77
MOL000492	(+)-catechin	54.83	0.24
MOL010921	estrone	53.56	0.32
MOL004908	Glabridin	53.25	0.47
MOL003295	(+)-pinoresinol monomethyl ether	53.08	0.57
MOL003290	(3R,4R)-3,4-bis[(3,4-dimethoxyphenyl)methyl]oxolan-2-one	52.3	0.48
MOL004497	Hippeastrine	51.65	0.62
MOL005911	5-Hydroxy-7,4'-dimethoxyflavanon	51.54	0.27
MOL013078	praeruptorin E	51.22	0.66
MOL007154	tanshinone iia	49.89	0.4
MOL010865	Naphthol aS-bl phosphate	49.88	0.45
MOL000096	(-)-catechin	49.68	0.24
MOL000354	isorhamnetin	49.6	0.31
MOL005921	quercetin 7-O-β-D-glucoside	49.57	0.27
MOL002915	Salvigenin	49.07	0.33
MOL000073	ent-Epicatechin	48.96	0.24
MOL004609	Areapillin	48.96	0.41
MOL000073	ent-Epicatechin	48.96	0.24
MOL013094	8-[(2R)-2,3-dihydroxy-3-methyl-butyl]-5,7-dimethoxy-coumarin	48.57	0.21
MOL004628	Octalupine	47.82	0.28
MOL005100	5,7-dihydroxy-2-(3-hydroxy-4-methoxyphenyl)chroman-4-one	47.74	0.27
MOL004624	Longikaurin A	47.72	0.53
MOL010863	3-acetyldeoxynivalenol	47.27	0.31
MOL013103	532-16-1	46.57	0.44
MOL013079	dl-praeruptorin a	46.46	0.53
MOL000098	quercetin	46.43	0.28
MOL004653	(+)-Anomalin	46.06	0.66
MOL004653	(+)-Anomalin	46.06	0.66
MOL010864	5,7-Dihydroxy-3',4',5'-trimethoxyflavon	46.01	0.37
MOL010485	EPA	45.66	0.21
MOL010861	Delta-D	45.66	0.48
MOL001942	isoimperatorin	45.46	0.23
MOL004373	Anhydroicaritin	45.41	0.44

MOL013100	(2S)-2-(1-hydroxy-1-methyl-ethyl)-9-[(2S,3R,4R,5S,6R)-3,4,5-trihydroxy-6-methylol-tetrahydropyran-2-yl]oxy-2,3-dihydrofuro[3,2-g]chromen-7-one	45.33	0.73
MOL000179	2-Hydroxyisoxypopyl-3-hydroxy-7-isopentene-2,3-dihydrobenzofuran-5-carboxylic	45.2	0.2
MOL002917	5,2',6'-Trihydroxy-7,8-dimethoxyflavone	45.05	0.33
MOL008206	Moslosooflavone	44.09	0.25
MOL003347	hyperforin	44.03	0.6
MOL003348	adhyperforin	44.03	0.61
MOL000449	Stigmasterol	43.83	0.76
MOL010482	WLN: 6OVR BVO6	43.74	0.24
MOL001749	ZINC03860434	43.59	0.35
MOL001490	bis[(2S)-2-ethylhexyl] benzene-1,2-dicarboxylate	43.59	0.35
MOL002879	Diop	43.59	0.39
MOL005922	Acanthoside B	43.35	0.77
MOL002897	epiberberine	43.09	0.78
MOL001002	ellagic acid	43.06	0.43
MOL004718	α -spinasterol	42.98	0.76
MOL004355	Spinasterol	42.98	0.76
MOL012588	7-[[[(1S,4aS,6R,8aR)-6-hydroxy-5,5,8a-trimethyl-2-methylene-decalin-1-yl]methoxy]coumarin	42.36	0.64
MOL001645	Linoleyl acetate	42.1	0.2
MOL003344	β -amyrin acetate	42.06	0.74
MOL007743	ZINC00391893	41.92	0.2
MOL000422	Kaempferol	41.88	0.24
MOL001951	Bergaptin	41.73	0.42
MOL007744	Chloranthalactone A	41.72	0.18
MOL004528	Icariin I	41.58	0.61
MOL002928	Oroxylin a	41.37	0.23
MOL002914	Eriodyctiol (flavanone)	41.35	0.24
MOL002910	Carthamidin	41.15	0.24
MOL003365	Lactucasterol	40.99	0.85
MOL007218	Remerin	40.75	0.52
MOL004798	delphinidin	40.63	0.28
MOL002032	DNOP	40.59	0.4
MOL000188	3 β -acetoxyaatractylone	40.57	0.22
MOL003281	20(S)-dammar-24-ene-3 β ,20-diol-3-acetate	40.23	0.82
MOL002644	Phellopterin	40.19	0.28
MOL002776	Baicalin	40.12	0.75
MOL002913	Dihydrobaicalin_qt	40.04	0.21
MOL002211	11,14-eicosadienoic acid	39.99	0.2
MOL013081	Decussine	39.83	0.65
MOL000525	Norwogonin	39.4	0.21
MOL010415	11,13-Eicosadienoic acid, methyl ester	39.28	0.23
MOL013077	Decursin	39.27	0.38
MOL000184	NSC63551	39.25	0.76
MOL002926	dihydrooroxylin A	38.72	0.23
MOL004492	Chrysanthemaxanthin	38.72	0.58
MOL005918	Phenanthrone	38.7	0.33
MOL003578	Cycloartenol	38.69	0.78
MOL013083	Skimmin (8CI)	38.35	0.32

MOL005884	Patchoulan 1,12-diol	38.17	0.25
MOL012266	Rivularin	37.94	0.37
MOL000953	CLR	37.87	0.68
MOL005916	Irisolidone	37.78	0.3
MOL007214	(+)-Leucocyanidin	37.61	0.27
MOL013076	(8S,9R)-9-hydroxy-8-(2-hydroxypropan-2-yl)-8,9-dihydrofuro[2,3-h]chromen-2-one	37.3	0.2
MOL005573	Genkwanin	37.13	0.24
MOL002908	5,8,2'-Trihydroxy-7-methoxyflavone	37.01	0.27
MOL002925	5,7,2',6'-Tetrahydroxyflavone	37.01	0.24
MOL000358	beta-sitosterol	36.91	0.75
MOL000085	beta-daucosterol_qt	36.91	0.75
MOL000088	beta-sitosterol 3-O-glucoside_qt	36.91	0.75
MOL000092	Daucosterin_qt	36.91	0.76
MOL000085	beta-daucosterol_qt	36.91	0.75
MOL000088	beta-sitosterol 3-O-glucoside_qt	36.91	0.75
MOL000359	Sitosterol	36.91	0.75
MOL008173	Daucosterol_qt	36.91	0.75
MOL000358	beta-sitosterol	36.91	0.75
MOL012593	isohumbertiol-3-o- $\{\alpha$ -L-rhamnopyranosyl(1 \rightarrow 4)- α -L-rhamnopyranosyl(1 \rightarrow 2)- $[\alpha$ -L-rhamnopyranosyl(1 \rightarrow 6)] $\}$ - β -D-glucopyranoside	36.75	0.59
MOL012245	5,7,4'-trihydroxy-6-methoxyflavanone	36.63	0.27
MOL002933	5,7,4'-Trihydroxy-8-methoxyflavone	36.56	0.27
MOL003305	Phillyrin	36.4	0.86
MOL004568	Engelitin	36.27	0.7
MOL000006	Luteolin	36.16	0.25
MOL003773	Mangiferolic acid	36.16	0.84
MOL012556	23-trans-p-coumarylformic acid	36.08	0.32
MOL010862	α -tocopheryl quinone	35.91	0.5
MOL005088	Nivalenol	35.68	0.28
MOL004540	Anemarsaponin C_qt	35.5	0.87
MOL004514	Timosaponin B III_qt	35.26	0.87
MOL001689	Acacetin	34.97	0.24
MOL001939	Alloisoimperatorin	34.8	0.22
MOL001941	Ammidin	34.55	0.22
MOL000522	Arctiin	34.45	0.84
MOL007213	Nuciferin	34.43	0.4
MOL002909	5,7,2,5-tetrahydroxy-8,6-dimethoxyflavone	33.82	0.45
MOL002372	(6Z,10E,14E,18E)-2,6,10,15,19,23-hexamethyltetracos-2,6,10,14,18,22-hexaene	33.55	0.42
MOL001506	Supraene	33.55	0.42
MOL002372	(6Z,10E,14E,18E)-2,6,10,15,19,23-hexamethyltetracos-2,6,10,14,18,22-hexaene	33.55	0.42
MOL007210	O-Nornuciferine	33.52	0.36
MOL002714	Baicalein	33.52	0.21
MOL012617	Torulene	33.49	0.55
MOL003315	3beta-Acetyl-20,25-epoxydammarane-24alpha-ol	33.07	0.79
MOL001956	Cnidilin	32.69	0.28
MOL007180	Vitamin-E	32.29	0.7

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	32.03	0.76
MOL004598	3,5,6,7-tetramethoxy-2-(3,4,5-trimethoxyphenyl)chromone	31.97	0.59
MOL000552	5,2'-Dihydroxy-6,7,8-trimethoxyflavone	31.71	0.35
MOL010922	Diisooctyl succinate	31.62	0.23
MOL004648	Troloxerutin	31.6	0.28
MOL012581	(4S,8R,9R)-4,8-bis(3,4-dihydroxyphenyl)-5,9-dihydroxy-4,8,9,10-tetrahydro-3H-pyrano[6,5-h]chromen-2-one	31.32	0.93
MOL002322	Isovitexin	31.29	0.72
MOL010846	Deoxynivalenol standard	31.16	0.25
MOL005923	3,23-dihydroxy-12-oleanen-28-oic acid	30.86	0.86
MOL010489	Resivit	30.84	0.27
MOL005030	Gondoic acid	30.7	0.2
MOL000173	Wogonin	30.68	0.23
MOL001458	Coptisine	30.67	0.86
MOL004542	Anemarsaponin E_qt	30.67	0.86
MOL004702	Saikosaponin c_qt	30.5	0.63
MOL012578	Cinchonain 1a	30.12	0.93
MOL000490	Petunidin	30.05	0.31
MOL007217	Leucodelphinidin	30.02	0.31
