

Table S1. Active ingredients of Yangyinjiedu (YYJD) herbal medicine.

ID	Compound	OB (%)	DL
MOL000483	(Z)-3-(4-hydroxy-3-methoxy-phenyl)-N-[2-(4-hydroxyphenyl)ethyl]acrylamide	118.35	0.26
MOL010387	3-o-beta-d-glucopyranosyl-(1-2)-[beta-d-xylopyranosyl-(1-3)]-beta-d-glucopyranosyl-(1-4)-galactopyranosyl-25(S)-spirost-5(6)-en-3beta,14alpo-diol Qt	104.58	0.79
MOL010395	4',5,7-trihydroxy-6-methyl-8-methoxy-homoisoflavanone	89.7	0.33
MOL000332	n-coumaroyltyramine	85.63	0.2
MOL010411	4',5,7-trihydroxy-6-methyl-homoisoflavanone	82.94	0.27
MOL009136	Peraksine	82.58	0.78
MOL006826	Chebulic acid	72	0.32
MOL003758	Iristectorigenin (9CI)	71.55	0.34
MOL003759	Iristectorigenin A	63.36	0.34
MOL010396	4',5,7-trihydroxy-6,8-dimethyl-homoisoflavanone	59.76	0.3
MOL002610	ZINC00035529	58.39	0.22
MOL010412	4'-methoxy-5,7-dihydroxy-6,8-dimethyl-homoisoflavanone	57.14	0.34
MOL009137	(R)-(6-methoxy-4-quinolyl)-[(2R,4R,5S)-5-vinylquinuclidin-2-yl]methanol	55.88	0.4
MOL003576	(1R,3aS,4R,6aS)-1,4-bis(3,4-dimethoxyphenyl)-1,3,3a,4,6,6a-hexahydrofuro[4,3-c]furan	52.35	0.62
MOL002605	11-Hydroxynumantenine	50.79	0.71
MOL002276	Senoside E Qt	50.69	0.61
MOL003753	Dihydrokaempferide	50.56	0.27
MOL000354	Isorhamnetin	49.6	0.31
MOL000351	Rhamnazin	47.14	0.34
MOL003769	Irolone	46.87	0.36
MOL009149	Cheilanthifoline	46.51	0.72
MOL000098	Quercetin	46.43	0.28
MOL001942	Isoimperatorin	45.46	0.23
MOL000179	2-Hydroxyisoxypopyl-3-hydroxy-7-isopentene-2,3-dihydrobenzofuran-5-carboxylic	45.2	0.2
MOL003742	Ardisianone A	44.22	0.25
MOL000449	Stigmasterol	43.83	0.76
MOL000186	Stigmasterol 3-O-beta-D-glucopyranoside Qt	43.83	0.76
MOL000449	Stigmasterol	43.83	0.76
MOL002609	Harmonyl	43.8	0.46
MOL003741	Anhydrobelachinal	43.57	0.78
MOL003754	Epianhydrobelachinal	43.57	0.78
MOL001002	Ellagic acid	43.06	0.43
MOL001040	(2R)-5,7-dihydroxy-2-(4-hydroxyphenyl)chroman-4-one	42.36	0.21
MOL000422	Kaempferol	41.88	0.24
MOL001951	Bergaptin	41.73	0.42
MOL000188	3β-acetoxyatractylone	40.57	0.22
MOL000184	NSC63551	39.25	0.76
MOL010408	Polygosides E Qt	38.73	0.78
MOL003578	Cycloartenol	38.69	0.78

MOL003542	8-Isopentenyl-kaempferol	38.04	0.39
MOL006376	7-Dehydrosigmasterol	37.42	0.75
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
MOL000296	Hederagenin	36.91	0.75
MOL000358	Beta-sitosterol	36.91	0.75
MOL003773	Mangiferolic acid	36.16	0.84
MOL000006	Luteolin	36.16	0.25
MOL001939	Alloisoimperatorin	34.8	0.22
MOL001941	Ammidin	34.55	0.22
MOL001956	Cnidilin	32.69	0.28
MOL003757	Iristectorene B	32.56	0.42
MOL002322	Isovitexin	31.29	0.72
MOL003743	Belachinal	31.24	0.64
MOL002619	Albaspidin AA	31.16	0.36
MOL001735	Dinatin	30.97	0.27
MOL009135	Ellipticine	30.82	0.28
MOL000173	Wogonin	30.68	0.23
MOL002614	Flavidin	30.1	0.26
MOL003744	Belamcandal	30.07	0.67
