

Table S3. Active ingredients of Chaihuqingzao (CHQZ) herbal medicine.

ID	Compound	OB (%)	DL
MOL007132	(2R)-3-(3,4-dihydroxyphenyl)-2-[(Z)-3-(3,4-dihydroxyphenyl)acryloyl]oxy-propionic acid	109.38	0.35
MOL011737	Divaricataacid	87	0.32
MOL005815	Citromitin	86.9	0.51
MOL007747	Chloranoside a_qt	84.11	0.23
MOL007742	Istanbulin-A	80.1	0.2
MOL004644	Sainfuran	79.91	0.23
MOL000011	(2R,3R)-3-(4-hydroxy-3-methoxy-phenyl)-5-methoxy-2-methylol-2,3-dihydropyrano[5,6-h][1,4]benzodioxin-9-one	68.83	0.66
MOL004580	cis-Dihydroquercetin	66.44	0.27
MOL005828	Nobiletin	61.67	0.52
MOL011732	Anomalin	59.65	0.66
MOL004328	Naringenin	59.29	0.21
MOL002610	Zinc00035529	58.39	0.22
MOL013187	Cubebin	57.13	0.64
MOL002605	11-Hydroxynumantenine	50.79	0.71
MOL011730	11-hydroxy-sec-o-beta-d-glucosylhamaudol_qt	50.24	0.27
MOL000354	Isorhamnetin	49.6	0.31
MOL004609	Areapillin	48.96	0.41
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
MOL000098	Quercetin	46.43	0.28
MOL007179	Linolenic acid ethyl ester	46.1	0.2
MOL004653	(+)-Anomalin	46.06	0.66
MOL001942	Isoimperatorin	45.46	0.23
MOL004373	Anhydroicaritin	45.41	0.44
MOL000179	2-Hydroxyisoxypopyl-3-hydroxy-7-isopentene-2,3-dihydrobenzofuran-5-carboxylic	45.2	0.2
MOL005996	2-O-methyl-3-O-β-D-glucopyranosyl platycogenate A	45.15	0.25
MOL007991	2-methoxy-9,10-dihydrophenanthrene-4,5-diol	44.97	0.18
MOL007165	10α-cucurbita-5,24-diene-3β-ol	44.02	0.74
MOL007175	karounidiol 3-o-benzoate	43.99	0.5
MOL000186	Stigmasterol 3-O-beta-D-glucopyranoside_qt	43.83	0.76
MOL000449	Stigmasterol	43.83	0.76
MOL002609	Harmonyl	43.8	0.46
MOL011749	Phelloptorin	43.39	0.28
MOL003485	Phthalic acid, isobutyl undecyl ester	43.33	0.36
MOL004718	α-spinasterol	42.98	0.76
MOL004355	Spinasterol	42.98	0.76
MOL001040	(2R)-5,7-dihydroxy-2-(4-hydroxyphenyl)chroman-4-one	42.36	0.21
MOL001645	Linoleyl acetate	42.1	0.2
MOL001494	Mandenol	42	0.19
MOL007743	ZINC00391893	41.92	0.2
MOL000422	Kaempferol	41.88	0.24

MOL007744	Chloranthalactone A	41.72	0.18
MOL003479	Cycloartenol acetate	41.11	0.8
MOL000188	3 β -acetoxyatractylone	40.57	0.22
MOL002644	Phellopterin	40.19	0.28
MOL002776	Baicalin	40.12	0.75
MOL006070	Robinin	39.84	0.71
MOL007514	Methyl icoso-11,14-dienoate	39.67	0.23
MOL013077	Decursin	39.27	0.38
MOL000184	NSC63551	39.25	0.76
MOL006026	Dimethyl 2-O-methyl-3-O-a-D-glucopyranosyl platycogenate A	39.21	0.25
MOL011753	5-O-Methylvisamminol	37.99	0.25
MOL006756	Schottenol	37.42	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
MOL000359	Sitosterol	36.91	0.75
MOL000358	beta-sitosterol	36.91	0.75
MOL000359	Sitosterol	36.91	0.75
MOL007172	7-oxo-dihydrokaro-unidiol	36.85	0.75
MOL005530	Hydroxygenkwanin	36.47	0.27
MOL003588	Prangenidin	36.31	0.22
MOL004568	Engelitin	36.27	0.7
MOL000006	Luteolin	36.16	0.25
MOL001689	Acacetin	34.97	0.24
MOL001941	Ammidin	34.55	0.22
MOL002883	Ethyl oleate (NF)	32.4	0.19
MOL007180	Vitamin E	32.29	0.7
MOL011747	Ledebouriellol	32.05	0.51
MOL004598	3,5,6,7-tetramethoxy-2-(3,4,5- trimethoxyphenyl)chromone	31.97	0.59
MOL011740	Divaricatol	31.65	0.38
MOL004648	Troxerutin	31.6	0.28
MOL002619	Albaspidin AA	31.16	0.36
MOL002881	Diosmetin	31.14	0.27
MOL000173	Wogonin	30.68	0.23
MOL004702	Saikosaponin c_qt	30.5	0.63
MOL007171	5-dehydrokarounidiol	30.23	0.77
MOL002614	Flavidin	30.1	0.26
MOL000490	Petunidin	30.05	0.31
