

Supplement Table 1. The main active ingredients of ZYDJD.

NO1	NO2	Compound name	OB	DL	Origin
MOL000358	A1	beta-sitosterol	36.91	0.75	Danggui
MOL000449	A2	Stigmasterol	43.83	0.76	Danggui
MOL001002	CS1	ellagic acid	43.06	0.43	Chishao
MOL001918	B1	paeoniflorgenone	87.59	0.37	Chishao
MOL001924	B2	paeoniflorin	53.87	0.79	Chishao
MOL002714	CS2	baicalin	33.52	0.21	Chishao
MOL002776	CS3	Baicalin	40.12	0.75	Chishao
MOL000358	A1	beta-sitosterol	36.91	0.75	Chishao
MOL000359	B3	sitosterol	36.91	0.75	Chishao
MOL004355	CS4	Spinasterol	42.98	0.76	Chishao
MOL000449	A2	Stigmasterol	43.83	0.76	Chishao
MOL000492	B4	(+)-catechin	54.83	0.24	Chishao
MOL006992	CS5	(2R, 3R)-4-methoxyl-distylin	59.98	0.3	Chishao
MOL006999	CS6	stigmast-7-en-3-ol	65.08	0.35	Chishao
MOL002883	B5	Ethyl oleate (NF)	32.4	0.19	Chishao
MOL005043	B6	campest-5-en-3beta-ol	37.58	0.71	Chishao
MOL001918	B1	paeoniflorgenone	87.59	0.37	Baishao
MOL001919	BS1	17-dihydroxy-4	43.56	0.53	Baishao
MOL001924	B2	paeoniflorin	53.87	0.79	Baishao
MOL000211	C1	Mairin	55.38	0.78	Baishao
MOL000358	A1	beta-sitosterol	36.91	0.75	Baishao
MOL000359	B3	sitosterol	36.91	0.75	Baishao
MOL000422	C2	kaempferol	41.88	0.24	Baishao
MOL000492	B4	(+)-catechin	54.83	0.24	Baishao
MOL001559	SY1	piperlonguminine	30.71	0.18	Shanyao
MOL001736	SY2	(-)-taxifolin	60.51	0.27	Shanyao
MOL000322	SY3	Kadsurenone	54.72	0.38	Shanyao
MOL005430	SY4	hancinone C	59.05	0.39	Shanyao
MOL005435	SY5	24-Methylcholest-5-enyl-3beta-O-glucopyranoside_qt	37.58	0.72	Shanyao
MOL005438	SY6	campesterol	37.58	0.71	Shanyao
MOL005440	D1	Isofucosterol	43.78	0.76	Shanyao
MOL005449	SY7	h-Met-h	43.83	0.76	Shanyao
MOL005458	SY8	Dioscoreside C_qt	36.38	0.87	Shanyao
MOL000546	SY9	diosgenin	80.88	0.81	Shanyao
MOL005465	SY10	AIDS180907	45.33	0.77	Shanyao
MOL000953	D2	CLR	37.87	0.68	Shanyao
MOL000359	B3	sitosterol	36.91	0.75	Shengdi
MOL000449	A2	Stigmasterol	43.83	0.76	Shengdi
MOL000358	A1	beta-sitosterol	36.91	0.75	Nvzhenzi
MOL000422	C2	kaempferol	41.88	0.24	Nvzhenzi
MOL000006	NZZ1	luteolin	36.16	0.25	Nvzhenzi
MOL000098	E1	quercetin	46.43	0.28	Nvzhenzi
MOL000211	C1	Mairin	55.38	0.78	Danpi
MOL000359	B3	sitosterol	36.91	0.75	Danpi
MOL000422	C2	kaempferol	41.88	0.24	Danpi
MOL000492	B4	(+)-catechin	54.83	0.24	Danpi
MOL007374	DP1	5-[[5-(4-methoxyphenyl)-2-furyl]methylene]barbituric acid	65.31	0.35	Danpi
MOL000098	E1	quercetin	46.43	0.28	Fuling
MOL000273	FL1	16-dihydroxy-4	30.93	0.81	Fuling
MOL000275	FL2	trametenolic acid	38.71	0.8	Fuling
MOL000279	FL3	Cerevisterol	37.96	0.77	Fuling
MOL000282	FL4	ergosta-7, 22E-dien-3beta-ol	43.51	0.72	Fuling
MOL000283	FL5	Ergosterol peroxide	40.36	0.81	Fuling
MOL000296	FL6	hederagenin	36.91	0.75	Fuling
MOL003152	XD1	Gentisin	64.06	0.21	Xuduan
MOL000358	A1	beta-sitosterol	36.91	0.75	Xuduan
MOL000359	B3	sitosterol	36.91	0.75	Xuduan
MOL009312	XD2	(E, E)-3, 5-Di-O-caffeoylquinic acid	48.14	0.68	Xuduan
MOL009323	XD3	Sylvestroside III_qt	56.47	0.43	Xuduan
MOL001558	TSZ1	sesamin	56.55	0.83	Tusizi
MOL000184	TSZ2	NSC63551	39.25	0.76	Tusizi
MOL000354	TSZ3	isorhamnetin	49.6	0.31	Tusizi
MOL000358	A1	beta-sitosterol	36.91	0.75	Tusizi
MOL000422	C2	kaempferol	41.88	0.24	Tusizi
MOL005043	B6	campest-5-en-3beta-ol	37.58	0.71	Tusizi
MOL005440	D1	Isofucosterol	43.78	0.76	Tusizi
MOL005944	TSZ4	matrine	63.77	0.25	Tusizi
MOL000953	D2	CLR	37.87	0.68	Tusizi
MOL000098	E1	quercetin	46.43	0.28	Tusizi
MOL000359	B3	sitosterol	36.91	0.75	Shanzhuyu
MOL005530	SDY1	Hydroxygenkwanin	36.47	0.27	Shanzhuyu
MOL005481	SDY2	2, 6, 10, 14, 18-pentamethylcosa-2, 6, 10, 14, 18-pentaene	33.4	0.24	Shanzhuyu
MOL008457	SDY3	Tetrahydroalstonine	32.42	0.81	Shanzhuyu
MOL002883	B5	Ethyl oleate (NF)	32.4	0.19	Shanzhuyu
MOL003137	SZY4	Leucanthoside	32.12	0.78	Shanzhuyu
MOL001771	SZY5	poriferast-5-en-3beta-ol	36.91	0.75	Shanzhuyu
MOL000358	A1	beta-sitosterol	36.91	0.75	Shanzhuyu
MOL005503	SZY6	Cornudentanone	39.66	0.33	Shanzhuyu
MOL001494	SZY7	Mandenol		42 0.19	Shanzhuyu
MOL002879	SZY8	Diop	43.59	0.39	Shanzhuyu
MOL000449	A2	Stigmasterol	43.83	0.76	Shanzhuyu
MOL001495	SZY9	Ethyl linolenate	46.1	0.2	Shanzhuyu
MOL005531	SZY10	Telocinobufagin	69.99	0.79	Shanzhuyu