

Supplementary Table 1 Effective active ingredients of herbs in Xuanshen decoction

No.	MOL ID	Ingredients	CAS id	OB (%)	DL
1	MOL00035 8	Beta-Sitosterol	83-46-5	36.913 9	0.7 1
2	MOL00765 8	14-deoxy-12(R)-sulfoandrogra pholide	None	62.569 1	0.4 2
3	MOL00281 3	Aucubin	479-98-1	35.559 9	0.3 3
4	MOL00192 5	Paeoniflorin_Qt	23180-57- 6	68.175 8	0.4
5	MOL00766 0	Scropolioside D_Qt	None	33.168 8	0.8 2
6	MOL00035 9	Sitosterol	83-46-5	36.913 9	0.7 5
7	MOL00222 2	Sugiol	511-05-7	36.113 5	0.2 8
8	MOL00715 4	Tanshinone Iia	568-72-9	49.887 3	0.4
9	MOL00656 4	(+)-Allomatrine	641-39-4	58.874 9	0.2 5
10	MOL00295 8	3'-Hydroxymelanettin	200391-95 -3	30.690 2	0.2 7
11	MOL00039 2	Formononetin	485-72-3	69.673 9	0.2 1
12	MOL00334 7	Hyperforin	11079-53- 1	44.033 2	0.6
13	MOL00000	Luteolin	491-70-3	36.162	0.2

	6			6	5
14	MOL00594	Matrine	519-02-8	63.774	0.2
	4			9	5
15	MOL00009	Quercetin	117-39-5	46.433	0.2
	8			3	8
16	MOL00366	Sophoranol	3411-37-8	67.319	0.2
	3			4	8
17	MOL00368	Sophoridine	6882-68-4	60.070	0.2
	0			3	5
18	MOL00041	Calycosin	20575-57-	47.751	0.2
	7		9	8	4
19	MOL00364	Sophojaponicin	30142-39-	41.505	0.7
	7		3	9	9
20	MOL00045	Phaseolin	22090-93-	78.200	0.7
	6		3	6	3
21	MOL00104	(2R)-5,7-Dihydroxy-2-(4-Hydroxyphenyl)Chroman-4-One	480-41-1	42.363	0.2
	0			3	1
22	MOL00321	Isoxanthohumol	521-48-2	56.810	0.3
	7			7	9
23	MOL00363	Oxynarcotine	None	56.742	0.6
	3			7	
24	MOL00367	Wighteone	51225-30-	42.796	0.3
	3		0	7	6
25	MOL00367	Sophoramine	6882-66-2	42.161	0.2
	6			9	5
26	MOL00494	(2R)-7-hydroxy-2-(4-hydroxyphenyl)chroman-4-one	578-86-9	71.123	0.1
	1				8
27	MOL00510	5,7-Dihydroxy-2-(3-Hydroxy-4-Methoxyphenyl)Chroman-4-	520-26-3	47.736	0.2
	0			4	7

		One			
28	MOL00656 1	(+)-14Alpha-Hydroxymatrine	None	35.726 5	0.2 9
29	MOL00656 3	(+)-9Alpha-Hydroxymatrine	None	32.045	0.2 9
30	MOL00656 5	Aids211310	17801-36- 4	68.676 8	0.2 5
31	MOL00656 9	(-)-14beta-hydroxymatrine	None	37.258	0.2 9
32	MOL00657 0	(-)-9Alpha-Hydroxysophoram ine	None	35.226 5	0.2 9
33	MOL00659 6	Glyceollin	57103-57- 8	97.274 7	0.7 6
34	MOL00658 2	5 α ,9 α -dihydroxymatrine	72362-00- 6	40.933 6	0.3 2
35	MOL00660 4	(2S)-7-Hydroxy-2-(4-Hydroxy phenyl)-5-Methoxy-8-(3-Meth ylbut-2-Enyl)Chroman-4-One	70872-29- 6	48.092 8	0.3 9
36	MOL00662 3	Kushenol,T	52483-01- 9	51.281 4	0.6 4
37	MOL00662 2	Kushenol O	None	42.405 3	0.7 6
38	MOL00662 8	(+)-Lupanine	550-90-3	52.707 2	0.2 4
39	MOL00663 0	Norartocarpetin	520-30-9	54.932 6	0.2 4
40	MOL00664 9	Sophranol	3411-37-8	55.416 6	0.2 8
41	MOL00662	Leachianone,G	None	60.971	0.4

	6			9	
42	MOL00665	(-)-Maackiain-3-O-Glucosyl-6'-		48.694	0.5
	0	O-Malonate	None	5	2
43	MOL00192		23180-57-	53.870	0.7
	4	Paeoniflorin	6	4	9
44	MOL00193		38642-49-	31.274	0.7
	0	Benzoyl Paeoniflorin	8	5	5
45	MOL00017			30.684	0.2
	3	Wogonin	632-85-9	6	3
46	MOL00004		61206-10-	54.066	0.2
	9	3 β -acetoxyatractylone	8	7	2
47	MOL00221			34.527	0.2
	9	Atropine	51-55-8	9	1
48	MOL00044			43.829	0.7
	9	Stigmasterol	83-48-7	9	6
49	MOL00009			36.913	0.7
	2	Daucosterin_Qt	474-58-8	9	6
50	MOL00009			36.913	0.7
	4	Daucosterol_Qt	474-58-8	9	6
51	MOL00018			39.253	0.7
	4	Nsc63551	4736-55-4	6	6
52	MOL00018	Stigmasterol		43.829	0.7
	6	3-O-Beta-D-Glucopyranoside_	None	9	6
		Qt			
53	MOL00017	2-Hydroxyisoxypyrpyl-3-Hyd		45.199	
	9	roxy-7-Isopentene-2,3-Dihydr	None	1	0.2
		obenzofuran-5-Carboxylic			
54	MOL00042			41.882	0.2
	2	Kaempferol	520-18-3	2	4

55	MOL00100	Ellagic Acid	476-66-4	43.064	0.4
	2			6	3
56	MOL00620	Cyanin	523-42-2	47.420	0.7
	9			9	6
57	MOL01288	Citrostadienol	None	43.281	0.7
	8			3	9
58	MOL01325	5,2',5'-Trihydroxy-6,7,8-Trimet	None	37.494	0.4
	3	hoxylavone		7	3
59	MOL00291	5,2',6'-Trihydroxy-7,8-Dimeth	92519-93-	45.047	0.3
	7	oxylavone	2	4	3
60	MOL00021	Mairin	472-15-1	55.377	0.7
	1			1	8
61	MOL00585	3,7,8-Tri-O-Methylellagic Acid	124590-38	37.542	0.5
	8		-1	2	7
62	MOL00586	Methyl		48.068	0.6
	2	4,6-Di-O-Galloyl-Beta-D-Gluc	None	4	8
		opyranoside			
63	MOL00586	Daucostero_Qt	474-58-8	36.913	0.7
	9			9	5
64	MOL00054	Diosgenin	512-04-9	80.877	0.8
	6			9	1
65	MOL00526	Elymoclavine	548-43-6	72.871	0.2
	7			9	7
66	MOL00542	Hancinol	108864-50	64.013	0.3
	9		-2	3	7
67	MOL00032	Kadsurenone	95851-37-		0.3
	2		9	54.723	8
68	MOL00031	Denudatin B	87402-88-	61.472	0.3
	0		8	4	8

69	MOL00095	Cholesterol	80356-14-	37.873	0.6
	3		5	9	8
70	MOL00155	Piperlonguminine	CAS:5950	30.711	0.1
	9		-12-9	4	8
71	MOL00544	Isofucosterol	18472-36-	43.776	0.7
	0		1	4	6
72	MOL00546	Doradexanthin	None	38.155	0.5
	1			8	4
73	MOL00793	Diosbulbin B	20086-06-	43.011	0.7
	9		0		
74	MOL00978	Diosbulbin C	20086-07-	65.867	0.6
	9		1	3	
75	MOL00543	24-Methylcholest-5-Enyl-3Belt	None	37.576	0.7
	5	a-O-Glucopyranoside_Qt		8	2
76	MOL00226	Rhein		47.065	0.2
	8		478-43-3	2	8
77	MOL00079	Bicuculline		69.667	0.8
	1		485-49-4	5	8
78	MOL01206	Cimigenol		37.186	0.4
	2		3779-59-7	9	
79	MOL00357	Cycloartenol		38.685	0.7
	8		469-38-5	7	8
80	MOL00078	Adlumidine		66.548	0.8
	0		550-49-2	8	8
81	MOL01205	Tuberosine A	155159-01	102.66	0.3
	2		-6	7	4
82	MOL01205	Cimicifugic Acid	None	83.023	0.4
	3			3	5
83	MOL01202	7,8-Didehydrocimigenol	None	36.791	0.4

	3			7	
84	MOL00048 3	(Z)-3-(4-Hydroxy-3-Methoxy-Phenyl)-N-[2-(4-Hydroxyphenyl)Ethyl]Acrylamide	80510-09-4	118.34 8	0.2 6
85	MOL01199 9	24-Epi-Acerinol	None	31.311 2	0.4 2
86	MOL00035 4	Isorhamnetin	480-19-3	49.604 4	0.3 1
87	MOL00049 7	Licochalcone A	58749-22-7	40.789 7	0.2 9
88	MOL00145 4	Berberine	2086-83-1	36.861 2	0.7 8
89	MOL00432 8	Naringenin	480-41-1 67604-48-2	59.293 9	0.2 1
90	MOL00490 3	Liquiritin	551-15-5	65.690 1	0.7 4
91	MOL00582 8	Nobiletin	478-01-3	61.669 4	0.5 2
92	MOL00232 2	Isovitexin	38953-85-4 61838-34-4	31.294 6	0.7 2
93	MOL00490 4	Licopyranocoumarin	117038-80-9	80.36	0.6 5
94	MOL00491 7	Glycyroside	125310-04-5	37.250 3	0.7 9
95	MOL00488 5	Licoisoflavanone	66067-26-3	52.466 2	0.5 4
96	MOL00389	7-Methoxy-2-Methyl	19725-44-	42.564	0.2

	6	Isoflavone	1	7	
97	MOL00023	Pinocembrin	480-39-7	57.562	0.2
	0			5	
98	MOL00023	Jaranol	3301-49-3	50.828	0.2
	9			8	9
99	MOL00050	Vestitol	20879-05-	74.655	0.2
	0		4	2	1
100	MOL00179	4H-1-Benzopyran-4-one, 2,3-dihydro-7-hydroxy-2-(4-hy	578-86-9	32.762	0.1
	2	droxyphenyl)-		7	8
101	MOL00231	Glycyrol	23013-84-	90.775	0.6
	1		5	8	7
102	MOL00256	Medicarpin	32383-76-	49.219	0.3
	5		9	8	4
103	MOL00365	Lupiwighteone	104691-86	51.635	0.3
	6		-3	7	7
104	MOL00385	Isoramanone	4644-99-9	39.966	0.5
	1			9	1
105	MOL00480	(2S)-2-[4-Hydroxy-3-(3-Methyl but-2-Enyl)Phenyl]-8,8-Dimet	157414-03	31.787	0.7
	5	hyl-2,3-Dihydropyrano[2,3-F] Chromen-4-One	-4		2
106	MOL00480	Euchrenone	None	30.287	0.5
	6			3	7
107	MOL00480	Glyasperin B	142488-54	65.224	0.4
	8		-8	4	4
108	MOL00481	Glyasperin F	None	75.836	0.5
	0			8	4
109	MOL00481	Glyasperin C	142474-53	45.563	0.4

	1		-1	8	
110	MOL00481	Isotrifoliol	None	31.944	0.4
	4			8	2
111	MOL00481	(E)-1-(2,4-Dihydroxyphenyl)-3		39.616	0.3
	5	-(2,2-Dimethylchromen-6-Yl)P	None	9	5
		rop-2-En-1-One			
112	MOL00482	(2S)-6-(2,4-Dihydroxyphenyl)-		60.250	0.6
	4	2-(2-Hydroxypropan-2-Yl)-4-	None	4	3
		Methoxy-2,3-Dihydrofuro[3,2-			
		G]Chromen-7-One			
113	MOL00482	Semilicoisoflavone B	129280-33	48.777	0.5
	7		-7	6	5
114	MOL00482	Glepidotin A	42193-83-	44.721	0.3
	8		9	9	5
115	MOL00483	Phaseolinisoflavan	40323-57-	32.008	0.4
	3		7	1	5
116	MOL00483	Glypallichalcone	146763-58	61.597	0.1
	5		-8	1	9
117	MOL00483	8-(6-Hydroxy-2-Benzofuranyl)		58.437	0.3
	8	-2,2-Dimethyl-5-Chromenol	None	3	8
118	MOL00484	Licochalcone B	58749-23-	76.757	0.1
	1		8	4	9
119	MOL00484	Licochalcone G	None	49.255	0.3
	8				2
120	MOL00484	3-(2,4-Dihydroxyphenyl)-8-(1,		59.622	0.4
	9	1-Dimethylprop-2-Enyl)-7-Hy	None	5	3
		droxy-5-Methoxy-Coumarin			
121	MOL00485	Licoricone	51847-92-	63.578	0.4
	5		8	5	7

122	MOL00485	Gancaonin A	27762-99-8	51.075	0.4
123	MOL00485	Gancaonin B	124596-86-7	48.794	0.4
124	MOL00486	3-(3,4-Dihydroxyphenyl)-5,7-Dihydroxy-8-(3-Methylbut-2-Enyl)Chromone	129145-50-2	66.371	0.4
125	MOL00486	5,7-Dihydroxy-3-(4-Methoxyphenyl)-8-(3-Methylbut-2-Enyl)Chromone	129145-51-3	30.488	0.4
126	MOL00486	2-(3,4-Dihydroxyphenyl)-5,7-Dihydroxy-6-(3-Methylbut-2-Enyl)Chromone	129145-53-5	44.152	0.4
127	MOL00487	Glycyrin	66056-18-6	52.606	0.4
128	MOL00488	Licoisoflavone	66056-19-7	41.610	0.4
129	MOL00488	Licoisoflavone B	66056-30-2	38.928	0.5
130	MOL00489	Shinpterocarpin	157414-04-5	80.295	0.7
131	MOL00489	(E)-3-[3,4-Dihydroxy-5-(3-Methylbut-2-Enyl)Phenyl]-1-(2,4-Dihydroxyphenyl)Prop-2-En-1-One	None	46.267	0.3
132	MOL00490	3,22-Dihydroxy-11-Oxo-Delta(12)-Oleanene-27-Alpha-Methoxycarbonyl-29-Oic Acid	123914-44-3	34.319	0.5
133	MOL00490	Glyzaglabrin	None	61.068	0.3

	7			9	5
134	MOL00490	Glabridin	59870-68-	53.245	0.4
	8		7	1	7
135	MOL00491	Glabranin	41983-91-	52.895	0.3
	0		9	7	1
136	MOL00491	Glabrene	60008-03-	46.266	0.4
	1		9	9	4
137	MOL00491	1,3-Dihydroxy-9-Methoxy-6-Benzofurano[3,2-C]Chromenone	None	48.141	0.4
	3			5	3
138	MOL00491	1,3-Dihydroxy-8,9-Dimethoxy-6-Benzofurano[3,2-C]Chromenone	None	62.901	0.5
	4			4	3
139	MOL00491	Eurycarpin A	None	43.277	0.3
	5			3	7
140	MOL00492	(-)-Medicocarpin	None	40.994	0.9
	4				5
141	MOL00493	Sigmoidin-B	87746-47-	34.881	0.4
	5		2	1	1
142	MOL00494	(2S)-7-Hydroxy-2-(4-Hydroxyphenyl)-8-(3-Methylbut-2-Enyl)Chroman-4-One	31524-62-	36.565	0.3
	5		6	4	2
143	MOL00494	Isoglycyrol	23013-86-	44.699	0.8
	8		7	2	4
144	MOL00494	Isolicoflavonol	94805-83-	45.17	0.4
	9		1		2
145	MOL00495	1-Methoxyphaseollidin	None	69.981	0.6
	9				4
146	MOL00496	Quercetin Der.	4382-17-6	46.449	0.3

	1			4	3
147	MOL00496	3'-Hydroxy-4'-O-Methylglabridin	None	43.715	0.5
	6				7
148	MOL00497	3'-Methoxyglabridin	None	46.161	0.5
	4			5	7
149	MOL00497	2-[(3R)-8,8-Dimethyl-3,4-Dihydro-2H-Pyrano[6,5-F]Chromen-3-Yl]-5-Methoxyphenol	None	36.214	0.5
	8			3	2
150	MOL00498	Inflacoumarin A	158446-33	39.709	0.3
	0		-4	1	3
151	MOL00498	Icos-5-Enoic Acid	None	30.702	0.2
	5			9	
152	MOL00498	Kanzonol F	None	32.468	0.8
	8			3	9
153	MOL00498	6-Prenylated Eriodictyol	None	39.223	0.4
	9			8	1
154	MOL00499	7,2',4'-Trihydroxy-5-Methoxy-3-Arylcoumarin	— None	83.714	0.2
	0			4	7
155	MOL00499	7-Acetoxy-2-Methylisoflavone	3211-63-0	38.923	0.2
	1			3	6
156	MOL00499	8-Prenylated Eriodictyol	None	53.794	0.4
	3			8	
157	MOL00499	Gadelaidic Acid	506-31-0	30.702	0.2
	6			9	
158	MOL00500	Gancaonin G	126716-34	60.435	0.3
	0		-5	2	9
159	MOL00500	Gancaonin H	126716-35	50.103	0.7
	1		-6	7	8
160	MOL00500	Licoagrocarpin	None	58.813	0.5

	3			9	8
161	MOL00500	Glyasperins M	None	72.670	0.5
	7			8	9
162	MOL00500	Glycyrrhiza Flavonol A	None	41.275	0.6
	8			3	
163	MOL00501	18A-Hydroxyglycyrrhetic	17991-67-	41.161	0.7
	3	Acid	2	4	1
164	MOL00501	Xambioona	None	54.849	0.8
	8			2	7
