

Table S1 Effective components of *Inulae Flos* (Xuan-Fu-Hua) and *Rubia cordifolia* (Qian-Cao) in Xuan-Fu-Hua decoction documented in TCMSP database with OB higher than 30% and DL index greater than 0.18

Ingredient	Molecule name	Pubchem cid	Mol ID	MW	OB (%)	DL
Inulae Flos (Xuan-Fu-Hua)	luteolin	5280445	MOL000006	286.25	36.16	0.25
	quercetin	5280343	MOL000098	302.25	46.43	0.28
	isorhamnetin	5281654	MOL000354	316.28	49.6	0.31
	beta-sitosterol	222284	MOL000358	414.79	36.91	0.75
	amyrin Palmitate (β -amyrin palmitate)	13915599	MOL000363	665.26	32.68	0.3
	kaempferol	5280863	MOL000422	286.25	41.88	0.24
	[(3S,4aR,6aR,6aR,6bR,8aR,12S,12aR,14aR,14bR)-4,4,6a,6b,8a,12,14b-heptamethyl-11-methylene-1,2,3,4a,5,6,6a,7,8,9,10,12,12a,13,14,14a-hexadecahydricen-3-yl] acetate	13889352	MOL000596	468.84	43.08	0.74
	Chryseriol	5280666	MOL003044	300.28	35.85	0.27
	Pratensein	5281803	MOL003398	299.27	39.06	0.28
	Isoramanone (digipurpurogenin II)	68807316	MOL003851	348.53	39.97	0.51
	Tamarixetin	5281699	MOL004083	316.28	32.86	0.31
	inulicin	442263	MOL004089	308.41	30.12	0.22
	3-[(3aS,4R,5R,8aR)-4-hydroxy-5,7-dimethyl-3-methylene-2-oxo-4,5,8,8a-tetrahydro-3aH-cyclohepta[b]furan-6-yl]propyl acetate	36564	MOL004090	308.41	73.35	0.22
	[(3aR,4R,7aR)-5-[(1S)-4-acetoxy-1-methyl-butyl]-6-methyl-3-methylene-2-oxo-3a,4,7,7a-tetrahydrobenzofuran-4-yl] acetate	10360513	MOL004092	350.45	39.03	0.31
	Azaleatin	5281604	MOL004093	316.28	54.28	0.3
	Britanin	5315501	MOL004094	366.45	33.73	0.41
	epifriedelanol acetate	13688752	MOL004096	470.86	31.18	0.74
	Melilotoside	5280759	MOL004101	326.33	36.85	0.26
	Patuletin	5281678	MOL004112	332.28	53.11	0.34
	Rubia Cordifolia (Qian-Cao)	beta-sitosterol	222284	MOL000358	414.79	36.91
sitosterol		12303645	MOL000359	414.79	36.91	0.75
(2R,3R,4S)-4-(4-hydroxy-3-methoxy-phenyl)-7-methoxy-2,3-dimethylol-tetralin-6-ol		160521	MOL003283	360.44	66.51	0.39
Mollugin		124219	MOL005638	284.33	42.34	0.26
daucostero_qt		N/A	MOL005869	414.79	36.91	0.75
1,3-dimethoxy-2-carboxyanthraquinone		N/A	MOL006139	312.29	102.89	0.33
1,3-dihydroxy-2-hydroxymthylanthraquinone-3-O-xylosyl(1 \rightarrow 6)-glucoside_qt		N/A	MOL006141	284.28	71.27	0.27
Alizarin-2-methylether		80103	MOL006147	254.25	32.81	0.21
7-hydroxy-8-methyl-4-vinyl-9,10-dihydrophenanthrene-1-carboxylic acid		9993796	MOL006149	278.32	56.99	0.27
1-acetoxy-6-hydroxy-2-methylanthraquinone-3-O- α -rhamnosyl(1 \rightarrow 4)- α -glucoside		N/A	MOL006150	616.67	30.74	0.64
2'-hydroxymollugin		N/A	MOL006153	302.35	40.5	0.29
4-hydroxy-9,10-dioxoanthracene-2-carboxylic acid		179447	MOL006155	266.21	45.98	0.25
Alizarin		6293	MOL006160	240.22	32.67	0.19
Nordamnacanthal		160712	MOL006162	268.23	53.97	0.24
Pallasone		5318483	MOL006164	374.62	43.87	0.4
methyl 6-hydroxy-2,2-dimethyl-3,4-dihydrobenzo[h]chromene-5-carboxylate	10779560	MOL006167	286.35	51.09	0.25	
Henine	10163	MOL006170	270.25	77.12	0.24	
rubiprasin B	N/A	MOL006171	498.87	35.97	0.68	
Xyloidone	72734	MOL006174	240.27	31.61	0.18	

OB, oral bioavailability; DL, drug-like; MW, molecular weight; N/A, the molecule has no Pubchem Cid.