

Table 1. Predicted dose number based on *in silico* solubility and dose number based on experimentally determined solubility of AMCs

CHM	AMC	Standard dose (mg)	Predicted D ₀ at pH 7	Experimental D ₀ at pH 7	Solubility classification ^a
Banlangen	(R,S)- Goitrin	Max: 4.5	0.0031	0.0036 ¹	c
		Min: 2.7	0.0018	0.0018	c
Breviscapine	Scutellarin	Max: 45	0.0002	2.687 ²	fp
		Min: 27	0.0001	1.612	fp
Cinnamon	Cinnamaldehyde	Max: 7.5	0.01	0.0214 ³	c
		Min: 1.5	0.002	0.00429	c
Licorice	Glycyrrhizic acid	Max: 400	0.0016	0.32 ⁴	c
		Min: 200	0.0008	0.16	c
Ma-huang	Ephedrine hydrochloride	Max: 80	0.00032	0.00032 ⁵	c
		Min: 16	0.00064	0.000064	c
	Pseudoephedrine hydrochloride	Max: 80	0.00032	0.00016 ⁶	c
		Min: 16	0.00064	0.000032	c
Milkvetch Root	Astragaloside IV	Max: 12	1.2632	2.16 ⁷	c
		Min: 3.6	0.3789	0.649	c
Red sage	Tanshinone II _A	Max: 30	57.1429	500 ⁸	c
		Min: 20	38.0952	333.3	c
	Salvianolic acid B	Max: 450	0.0018	0.00402 ⁹	c
		Min: 300	0.0012	0.00279	c
Tang-kuei	Ferulic acid	Max: 6	0.000024	0.126 ¹⁰	c
		Min: 3	0.000012	0.063	c
Blister Beetle oral pill	Cantharidin	Max: 0.21	0.029	0.009423 ¹¹	c
		Min: 0.105	0.0145	0.004711	c
Fufang Danshen tablet	Tanshinone II _A	0.6	1.1429	10 ⁸	c
	Salvianolic acid B	15	0.0001	0.000134 ⁹	c
Ginkgo biloba leaf extract tablet	Quercetin	19.2	0.0404	4.47 ¹²	fp
	Kaempferol	19.2	0.1219	2.36 ¹²	fp
	Isorhamnetin	19.2	0.1506	67.96 ¹²	fp
	Bilobalide	4.8	0.0310	0.0138 ¹³	c
	Ginkgolide A	4.8	0.0031	0.0736 ¹³	c
	Ginkgolide B	4.8	0.0196	0.1885 ¹⁴	c
	Ginkgolide C	4.8	0.0175	0.040 ¹³	c

Moschus pill	Muscone	Max: 2	0.0727	0.0124 ¹⁵	c
		Min: 0.6	0.0218	0.00372	c
Notoginseng	Gensenoside	Max: 750	1000	0.1565 ¹⁶	fn
Total Saponins	Rg ₁	Min: 250	333.3	0.0521	fn
Pingxiao tablet	Strychnine	Max: 2.8	0.00303	0.000349 ¹⁷	c
		Min: 0.8	0.00086	0.00010	c
	Baicalin	Max: 44	0.00018	1.571 ¹⁸	fp
		Min: 18	0.00007	0.643	c
Qingkailing tablet	Cholic acid	Max: 31.2	0.0277	1.230 ¹⁹	fp
		Min: 10.4	0.0092	0.433	c
	Geniposide	Max: 2	0.0004	0.00008 ²⁰	c
		Min: 1	0.0002	0.00004	c
Shuanghuang-lian tablet	Chlorogenic acid	22	0.0001	0.00578 ²¹	c
	Baicalin	200	0.0008	7.143 ¹⁸	fp
Xueshuan	Anhydrous	48	0.0287	0.9648 ²²	c
Xinmaining capsule	Rutin				
Allicin tablet	Allicin	20	0.0031	0.0032 ²³	c
Andrographolide tablet	Andrographolide	Max: 150	0.1765	12.9 ²⁴	fp
		Min: 100	0.1176	8.65	fp
Asiaticosid tablet	Asiaticosid	12	32	0.48 ²⁵	fn
Butylphthalide capsule	Butylphthalide	200	6.1538	8 ²⁶	c
Extract of horse chestnut seeds tablet	Esculin	Max: 300	0.0207	0.774 ²⁷	c
		Max: 150	0.0103	0.387	c
Silybin	Silybin	Max: 200	421.053	16.56 ²⁸	c
Meglumine tablet	Meglumine	Min: 100	210.526	8.28	c

^aPredicted D_o comparison with Experimental D_o classification: c = correctly classified; fp = false positive classification; fn = false negative classification.

Table 2. Predicted Log P , Log $D_{6.0}$ and Caco-2 cell monolayer apical to basolateral permeability coefficient (P_{app}) of AMCs

AMC	Log P	Log $D_{6.0}$	P_{app} ($\times 10^6$ cm/s)	Permeability classification ^b	
				Log P based	Log $D_{6.0}$ based
Metoprolol (reference compound)	1.632		18 ²⁹		
Labetalol (reference compound)		-0.15	9.3 ³⁰		
Scutellarin	0.43	-3.19	0.95 ³¹	c	c
Quercitrin	0.58	0.26	0.79 ³²	c	fp
Liquiritin	0.28	0.27	0.54 ³³	c	fp
Ephedrine hydrochloride	1.08	-1.86	10.2 ^{34, 35}	c	fn
Pseudoephedrine hydrochloride	1.08	-1.86	16.1 ⁷	c	fn
Astragaloside IV	0.63	0.63	0.037 ³⁶	c	fp
Paeoniflorin	0.25	0.25	0.24 ³⁷	c	fp
Tanshinone II _A	4.93	4.93	29 ³⁸	c	c
Salvianolic acid B	2.14	-5.41	0.34 ³⁹	fp	c
Ferulic acid	0.96	-0.7	10.2 ⁴⁰	c	fn
Quercetin	2.08	1.78	3.9 ³²	fp	fp
Kaempferol	2.69	2.49	10.2 ³²	fp	c
Isorhamnetin	2.79	2.58	1.4 ⁴¹	fp	fp
Bilobalide	11.7	4.46	2.1 ⁴²	fp	fp
Ginkgolide A	-0.036	-0.04	0.81 ⁴²	c	fp
Ginkgolide B	2.07	2.07	11 ¹⁵	fp	c
Ginkgolide C	1.72	1.72	1.2 ⁴²	fp	fp
Gensenoside Rg ₁	1.5	1.5	0.26 ⁴³	c	fp
Notoginsenoside R ₁	1.35	1.35	0.088 ⁴⁴	c	fp
Strychnine	1.59	-0.74	26.4 ⁴⁵	fn	fn
Baicalin	1.43	-2.19	0.17 ³²	c	c
Geniposide	-2.08	-2.08	0.11 ⁴⁶	c	c
Chlorogenic acid	0.37	-2.25	1 ⁴⁷	c	c
Rutin	-0.9	-1.13	0 ³²	c	c
Andrographolide	0.42	0.42	11.4 ⁴⁸	c	c
Esculin	-1.31	-1.35	17.4 ⁴⁹	c	fn

^bLog P and Log $D_{6.0}$ comparison with Caco-2 permeability coefficient classification: c = correctly classified; fp = false positive classification; fn = false negative classification.

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