Supplementary material

Preparative separation of structural isomeric pentacyclic triterpene oleanolic acid and ursolic acid from natural products by pH-zone-refining countercurrent chromatography

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Table 1 Partition coefficient of oleanolic acid and ursolic acid in the investigated two-phase solvent systems for pH-refining-zone countercurrent chromatography

Solvent systems			**Partition coefficient (*K*)**	
			OA	UA
n-hexane:ethyl acetate:methanol:water	5:5:2:8	K_{base}	4.964	4.853
		K_{acid}	168.484	146.25
	6:4:2:8	K_{base}	3.036	3.357
		K_{acid}	28.824	267.457
	10:0:2:8	K_{base}	0.593	0.913
		K_{acid}	126.384	179.171
	7:3:3:7	K_{base}	1.540	1.530
		K_{acid}	159.302	165.035
	9:1:3:7	K_{base}	0.380	0.324
		K_{acid}	139.021	147.409
	10:0:3:7	K_{base}	0.127	0.187
		K_{acid}	100.778	120.866
	4:6:4:6	K_{base}	0.415	0.403
		K_{acid}	76.750	75.420
	5:5:4:6	K_{base}	0.407	0.479
		K_{acid}	73.495	74.978
	6:4:4:6	K_{base}	0.3101	0.324
		K_{acid}	76.514	82.086
	7:3:4:6	K_{base}	0.276	0.303
		K_{acid}	66.477	84.286
methyl *tert*-butyl ether-tetrahydrofuran-water	1:0:1	K_{base}	2.96	3.301
		K_{acid}	125.046	182.047
	4:1:5	K_{base}	2.125	2.167
		K_{acid}	242.701	129.449
	2:2:3	K_{base}	0.369	0.3214
		K_{acid}	114.656	174.573
	6:3:8	K_{base}	2.577	2.461
		K_{acid}	34.545	55.271
methyl *tert*-butyl ether-acetonitrile-wate	4:1:5	K_{base}	0.422	0.395
		K_{acid}	225.88	312.046
	2:2:3	K_{base}	0.844	0.7398
		K_{acid}	34.067	31.839
	6:3:8	K_{base}	0.3387	0.3045
		K_{acid}	16.9217	26.8043
chloroform-methanol-water	4:3:2	K_{base}	0.2599	0.282
		K_{acid}	141.94	146.25
	4:3.5:2	K_{base}	0.175	0.183
		K_{acid}	101.381	72.303

	13:7:4	K_{base}	0.361	0.359
		K_{acid}	129.465	109.561
	10:8:4	K_{base}	0.4393	0.4613
		K_{acid}	29.923	28.4028
	2:2:1	K_{base}	0.107	0.113
		K_{acid}	41.031	51.573
chloroform-methanol-*n*-butanol-water	4:3:0.5:2	K_{base}	1.72	1.624
		K_{acid}	30.301	31.296
n-hexane-dichloromethane-methanol-water	7:3:4:6	K_{base}	0.035	0.04
		K_{acid}	7.637	6.725
	7:3:3:7	K_{base}	0.0669	0.06716
		K_{acid}	19.803	18.5536
	7:3:2:8	K_{base}	0.0726	0.0938
		K_{acid}	35.4918	47.841
	6:4:2:8	K_{base}	0.1536	0.1703
		K_{acid}	40.375	41.5388

Note: K_{acid} was determined with the biphasic solvent system added with 10 mmol/L of trifluoroacetic acid in the organic phase, and K_{base} was determined with the biphasic solvent system added with 10 mmol/L of ammonia (with 25%-28% NH_3) in the aqueous phase.

Table 2 Partition coefficient of oleanolic acid and ursolic acid in the investigated two-phase solvent systems for coventional countercurrent chromatography

Solvent systems	K_{OA}	K_{UA}	**α**
n-hexane-dichloromethane-methanol-1% acetic acid water(v/v, 9:1:6:4)	3.782	4.174	1.103
n-hexane-dichloromethane-methanol-1% acetic acid water (v/v, 9:1:7:3)	1.560	1.644	1.054
n-hexane-dichloromethane-methanol-1% acetic acid water (v/v, 7:3:7:3)	2.698	2.007	1.215
n-hexane-dichloromethane-methanol-1% acetic acid water (v/v, 8:2:7:3)	2.164	2.007	1.078
n-hexane-dichloromethane-methanol-1% acetic acid water(v/v, 7:3:8:2)	0.830	0.727	1.133
n-hexane-ethyl acetate-methanol-1% acetic acid water(v/v, 7:3:6:4)	1.812	1.933	1.067
n-hexane-ethyl acetate-methanol-1% acetic acid water(v/v, 7:3:5:5)	2.066	2.233	1.081
n-hexane-ethyl acetate-methanol-1% acetic acid water(v/v, 7:3:4:6)	2.509	2.775	1.106