

Supplemental Table 3 The chemical composition of Yiqi Huoxue Recipe under negative ion mode

NO.	Component Name	Area	Retention		Precursor Mass	Found At Mass	Mass		Isotope Ratio
			Time	Formula			Error (ppm)	Library Score	
1	Histidine	32090	1.07	C ₆ H ₉ N ₃ O ₂	154.062	154.062	-1.1	82.2	0.7
2	Arginine	111200	1.07	C ₆ H ₁₄ N ₄ O ₂	173.104	173.1042	-1.1	88.5	4.3
3	Citrulline	42640	1.15	C ₆ H ₁₃ N ₃ O ₃	174.088	174.0885	0.4	97.7	2.6
4	Sorbitol	69100	1.15	C ₆ H ₁₄ O ₆	181.072	181.0716	-0.9	91.2	3.4
5	D-(+)-Glucose	208600	1.21	C ₆ H ₁₂ O ₆	179.056	179.0562	0.2	71	2.8
6	Citric acid	3341000	1.85	C ₆ H ₈ O ₇	191.02	191.0196	-0.9	98.4	2.3
7	Succinic acid	110100	2.43	C ₄ H ₆ O ₄	117.019	117.0194	0.8	91.5	0.3
8	Adenosine	16160	2.65	C ₁₀ H ₁₃ N ₅ O ₄	266.089	266.0892	-1	94.7	3.2
9	Guanosine	451400	2.8	C ₁₀ H ₁₃ N ₅ O ₅	282.084	282.0841	-1	99.2	6.6
10	Rehmannioside D +HCOOH	695800	3.58	C ₂₇ H ₄₂ O ₂₀ .HCOOH	731.225	731.2245	-0.9	98.7	13.1
11	Phenprobamate	118900	3.69	C ₉ H ₁₁ NO ₂	164.072	164.0715	-0.9	99.4	4.5
12	Geniposidic acid	247200	4.31	C ₁₆ H ₂₂ O ₁₀	373.114	373.1137	-1	97.4	8.1
13	Neochlorogenic acid	1132000	4.9	C ₁₆ H ₁₈ O ₉	353.088	353.0875	-0.9	97.6	8

14	8-Epiloganic acid	204600	5.13	C ₁₆ H ₂₄ O ₁₀	375.13	375.1295	-0.4	98.4	5.7
15	L-Tryptophan	199000	5.14	C ₁₁ H ₁₂ N ₂ O ₂	203.083	203.0824	-0.8	97.3	3.5
16	Vitexin	10600000	5.99	C ₂₁ H ₂₀ O ₁₀	431.098	431.0982	-0.5	80.1	8.9
17	Quinic acid	333200	6.06	C ₇ H ₁₂ O ₆	191.056	191.056	-0.3	96.2	2.9
18	Fraxin	8161	6.69	C ₁₆ H ₁₈ O ₁₀	369.083	369.0825	-0.7	96.1	1.6
19	Caffeic acid	209200	6.7	C ₉ H ₈ O ₄	179.035	179.0348	-1	72.9	2.4
20	Puerarin	37290000	6.92	C ₂₁ H ₂₀ O ₉	415.103	415.1029	-1.3	98.2	9.8
21	3,5-Dicaffeoyl quinic acid	94140	7.49	C ₂₅ H ₂₄ O ₁₂	515.119	515.119	-0.9	97.4	6
22	Echinacoside	297800	7.64	C ₃₅ H ₄₆ O ₂₀	785.251	785.2498	-1.4	99.1	15.4
23	Daidzin +HCOOH	10400000	7.97	C ₂₁ H ₂₀ O ₉ .HCOOH	461.109	461.1083	-1.4	100	10
24	Calycosin-7-o-glucoside +HCOOH	2432000	9.01	C ₂₂ H ₂₂ O ₁₀ .HCOOH	491.119	491.1191	-0.9	99.3	11.6
25	Ferulic Acid	677400	9.1	C ₁₀ H ₁₀ O ₄	193.051	193.0503	-1.8	91.4	4.7
26	Acteoside; Verbascoside; Kusaginin	201200	9.53	C ₂₉ H ₃₆ O ₁₅	623.198	623.1976	-0.9	98.4	11.2
27	Diosmetin	22480	10.64	C ₁₆ H ₁₂ O ₆	299.056	299.0559	-0.8	83	5.2
28	4-Hydroxybenzoic acid	87160	11.18	C ₇ H ₆ O ₃	137.024	137.0243	-0.9	100	2.5
29	Ononin +HCOOH	3132000	12.1	C ₂₂ H ₂₂ O ₉ .HCOOH	475.125	475.1243	-0.7	99.2	10.9
30	Cistanoside D +HCOOH	1781	12.25	C ₃₁ H ₄₀ O ₁₅ .HCOOH	697.235	697.2318	-4.5	98.6	5.7

31	Daidzein	3526000	12.29	C ₁₅ H ₁₀ O ₄	253.051	253.0505	-0.6	98	6.2
32	Isoliquiritigenin	29410	12.58	C ₁₅ H ₁₂ O ₄	255.066	255.0662	-0.5	92.2	3.9
33	Astragaloside I +HCOOH	80910	12.64	C ₄₅ H ₇₂ O ₁₆ .HCOOH	913.48	913.4795	-0.8	92.9	15.6
34	Epimeredinoside A	72390	12.95	C ₃₁ H ₄₀ O ₁₅	651.229	651.2289	-0.8	87.4	13.5
35	Calycosin	1475000	13.13	C ₁₆ H ₁₂ O ₅	283.061	283.061	-0.6	98.1	7.6
36	Isomucronulatol-7-O-glucoside	364800	13.34	C ₂₃ H ₂₈ O ₁₀	463.161	463.1605	-0.9	97	11.4
37	Formononetin	375200	13.54	C ₁₆ H ₁₂ O ₄	267.066	267.066	-1	74.1	8
38	3-Hydroxy-9,10-Dimethoxypterocarpan	28120	14.06	C ₁₇ H ₁₆ O ₅	299.092	299.092	-1.8	85.8	0.8
