

SUPPLEMENTARY MATERIAL

Analysis of Chemical Constituents of Miao Ethnomedicine Heiguteng Zhuifeng Huoluo Capsule (HZFC) and Discovery of Active Substances in the Treatment of Rheumatoid Arthritis

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Table S1 Retention time, mass spectrometry information and identification results of chemical constituents in HZFC

No.	Name of compound	Molecular formula	Retention time(min)	M/z	Mass error	Ms/ms	Type the parent nucleus	Main source
1	Citric acid	C ₆ H ₈ O ₇	0.72	192.027	4.2	155.955	Organic acid	<i>Lysimachia paridiformis</i> var. <i>stenophylla</i> Franch.
2	Quinic acid	C ₆ H ₈ O ₇	0.87	192.027	4.2	155.955	Organic acid	<i>Lysimachia paridiformis</i> var. <i>stenophylla</i> Franch.
3	Uridine	C ₉ H ₁₂ N ₂ O ₆	0.89	244.0695	-4.5	111.019	Glycoside	<i>Lysimachia paridiformis</i> var. <i>stenophylla</i> Franch.
4	Guanosine	C ₁₀ H ₁₃ N ₅ O ₅	0.99	283.0917	1.6	150.0423	Glycoside	<i>Lysimachia paridiformis</i> var. <i>stenophylla</i> Franch.
5	Sinomenine N-oxide rhamnoside	C ₂₅ H ₃₃ NO ₉	2.12	491.2155	-0.6	346.1658, 330.171, 299.129, 28 1.15	Alkaloids	<i>Sinomenium acutum</i> (Thunb.) Rehder & E.H.Wilson
6	Protocatechuate	C ₇ H ₆ O ₄	2.18	154.0266	0.7	109.0297	Organic acid	<i>Periploca forrestii</i> Schltr.
7	Higenamine glucoside	C ₂₂ H ₂₇ NO ₈	2.26	433.1737	-2.1	270.1116, 162.0572	Alkaloids	<i>Sinomenium acutum</i> (Thunb.) Rehder & E.H.Wilson
8	Higenamine glucoside isomer	C ₂₂ H ₂₇ NO ₈	2.43	433.1737	-2.1	270.1116, 162.0572	Alkaloids	<i>Sinomenium acutum</i> (Thunb.) Rehder & E.H.Wilson
9	Hydroxytyrosol glucoside	C ₁₄ H ₂₀ O ₈	2.83	316.1115	3.5	153.0582	Phenols	<i>Periploca forrestii</i> Schltr.
10	Neochlorogenic acid	C ₁₆ H ₁₈ O ₉	3.2	354.0951	0.6	191.0547, 179.0352, 173.0465	Organic acid	<i>Periploca forrestii</i> Schltr.
11	Cephatonine glucoside	C ₂₆ H ₃₅ NO ₁₀	3.4	521.2261	1.3	476.1898, 360.1814, 314.1373	Glycoside	<i>Periploca forrestii</i> Schltr.
12	Norlaudanine glucoside	C ₂₅ H ₃₃ NO ₉	3.48	491.2155	-0.6	476.1899, 330.171, 316.1606	Glycoside	<i>Sinomenium acutum</i> (Thunb.) Rehder & E.H.Wilson
13	3,4-dihydroxybenzaldehyde	C ₇ H ₆ O ₃	3.64	138.0317	7.3	/	Depsides	<i>Lysimachia paridiformis</i> var. <i>stenophylla</i> Franch.
14	Higenamine	C ₁₆ H ₁₇ NO ₃	4.14	271.1208	-4	255.1031, 237.0916	Alkaloids	<i>Sinomenium acutum</i> (Thunb.) Rehder & E.H.Wilson
15	1-O-sinapoyl glucoside	C ₁₇ H ₂₂ O ₁₀	4.32	386.1213	-0.1	223.0611, 179.0708	Phenylpropanoids	<i>Periploca forrestii</i> Schltr.
16	Nor-sinomenine glucoside	C ₂₄ H ₃₁ NO ₉	4.43	477.1999	5.6	448.1972, 316.1533, 286.1431	Alkaloids	<i>Sinomenium acutum</i> (Thunb.) Rehder & E.H.Wilson
17	Acutumidine	C ₁₈ H ₂₂ NO ₆ Cl	4.51	383.1136	-4.6	348.1445, 341.0813, 305.1007	Alkaloids	<i>Sinomenium acutum</i> (Thunb.) Rehder & E.H.Wilson
18	Disinomenine	C ₃₈ H ₄₄ N ₂ O ₈	4.61	656.3098	-2.6	332.1855, 329.1241	Alkaloids	<i>Sinomenium acutum</i> (Thunb.) Rehder & E.H.Wilson
19	Chlorogenic acid	C ₁₆ H ₁₈ O ₉	4.77	354.0951	0.6	191.0547, 179.0352, 173.0465	Phenylpropanoids	<i>Periploca forrestii</i> Schltr.
20	Sinomenine	C ₁₉ H ₂₃ NO ₄	4.81	329.1627	2.4	255.1031, 241.0845, 239.0712	Alkaloids	<i>Sinomenium acutum</i> (Thunb.) Rehder & E.H.Wilson
21	Cryptochlorogenic	C ₁₆ H ₁₈ O ₉	5.15	354.0951	0.6	191.0547, 179.0352, 173.0465	Phenylpropanoids	<i>Periploca forrestii</i> Schltr.
22	Acutumine	C ₁₉ H ₂₄ NO ₆ Cl	5.25	397.1292	-5.3	362.1611, 341.0793, 323.0671, 305.1038, 287.0923, 273.0769	Alkaloids	<i>Sinomenium acutum</i> (Thunb.) Rehder & E.H.Wilson
23	Nor-sinomenine	C ₁₈ H ₁₉ NO ₄	5.37	313.1314	5.4	298.1068, 283.0846	Alkaloids	<i>Sinomenium acutum</i> (Thunb.) Rehder & E.H.Wilson
24	Deosinomenine glucoside	C ₂₅ H ₃₄ NO ₈	5.55	475.1842	3.4	314.1772, 269.1183	Alkaloids	<i>Sinomenium acutum</i> (Thunb.) Rehder &

									E.H.Wilson
25	Sibiricose A6	C ₂₃ H ₃₂ O ₁₅	5.93	548.1741	-0.1	/	Glycoside	<i>Lysimachia paridiformis</i> var. <i>stenophylla</i> Franch.	
						362.1611, 341.0793,		<i>Sinomenium acutum</i> (Thunb.) Rehder &	
26	Dauricumine	C ₁₉ H ₂₄ NO ₆ Cl	6.21	397.1292	-5.3	323.0671, 305.1038,	Alkaloids	E.H.Wilson	
						287.0923, 273.0769		<i>Sinomenium acutum</i> (Thunb.) Rehder &	
27	2,2'-disinomenine	C ₃₈ H ₄₄ N ₂ O ₈	6.25	656.3098	-2.6	332.1855, 329.1241	Alkaloids	E.H.Wilson	
								<i>Sinomenium acutum</i> (Thunb.) Rehder &	
28	Tuduranine	C ₁₈ H ₁₉ NO ₃	6.37	297.1365	4.7	269.1183	Alkaloids	E.H.Wilson	
								<i>Sinomenium acutum</i> (Thunb.) Rehder &	
29	Magnoflorine	C ₂₀ H ₂₄ NO ₄ ⁺	6.39	342.1705	5.9	325.1321	Alkaloids	E.H.Wilson	
						298.1457, 270.1498,		<i>Sinomenium acutum</i> (Thunb.) Rehder &	
30	Isosinomenine	C ₁₉ H ₂₃ NO ₄	6.98	329.1627	2.4	255.1031	Alkaloids	E.H.Wilson	
						353.0891, 335.0762,		<i>Periploca forrestii</i> Schltr.	
31	3-O-caffeoyl--O-sinapoylquinic acid	C ₂₇ H ₂₈ O ₁₃	7.2	560.1529	-0.1	191.0547	Phenylpropanoids		
						579.2101, 417.1537,		<i>Periploca forrestii</i> Schltr.	
32	Syringaresinol di-O-glucoside	C ₃₄ H ₄₆ O ₁₈	7.95	742.2684	0.4	357.1336	Phenylpropanoids		
								<i>Lysimachia paridiformis</i> var. <i>stenophylla</i> Franch.	
33	Rutin	C ₂₇ H ₃₀ O ₁₆	8.12	610.153	2	463.0911	Flavonoid		
								<i>Sinomenium acutum</i> (Thunb.) Rehder &	
34	Corydine methyl ether	C ₂₁ H ₂₅ NO ₄	8.24	355.1784	-2.8	311.1271,296.1035,279.1016	Alkaloids	E.H.Wilson	
								<i>Periploca forrestii</i> Schltr.	
35	Quercetin 3-O-glucoside	C ₂₁ H ₂₀ O ₁₂	8.3	464.095	0.9	300.0287	Flavonoid		
								<i>Sinomenium acutum</i> (Thunb.) Rehder &	
36	Stepharanine	C ₁₉ H ₁₈ NO ₄	8.62	324.1236	-0.1	309.0984,294.0753,266.0823	Alkaloids	E.H.Wilson	
								<i>Lysimachia paridiformis</i> var. <i>stenophylla</i> Franch.	
37	Kaempferol-3-O-rutinoside	C ₂₇ H ₃₀ O ₁₅	9.21	448.1006	0.5	285.0466	Flavonoid		
								<i>Periploca forrestii</i> Schltr.	
38	Isochlorogenic acid B	C ₂₅ H ₂₄ O ₁₂	8.99	516.1268	3.5	353.0891,191.0576,179.0352	Organic acid		
								<i>Periploca forrestii</i> Schltr.	
39	Isochlorogenic acid C	C ₂₅ H ₂₄ O ₁₂	9.14	516.1268	3.5	353.0891,191.0576,179.0352	Organic acid		
								<i>Lysimachia paridiformis</i> var. <i>stenophylla</i> Franch.	
40	Astragalin	C ₂₁ H ₂₀ O ₁₁	9.21	448.1006	0.5	285.0466	Flavonoid		
								<i>Lysimachia paridiformis</i> var. <i>stenophylla</i> Franch.	
41	Quercitrin	C ₂₁ H ₂₀ O ₁₁	9.28	448.1006	0.5	301.0335	Flavonoid		
								<i>Lysimachia paridiformis</i> var. <i>stenophylla</i> Franch.	
42	Syringaresinol di-o-glucoside isomer	C ₃₄ H ₄₆ O ₁₈	9.54	742.2684	0.4	579.2101,417.1537,357.1336	Phenylpropanoids		
								<i>Periploca forrestii</i> Schltr.	
43	Syringaresinol 4-O-glucoside	C ₂₈ H ₃₆ O ₁₃	9.69	580.2156	4	417.1537,357.1336	Phenylpropanoids		
								<i>Sinomenium acutum</i> (Thunb.) Rehder &	
44	Pseudocolumbamine	C ₂₀ H ₂₀ NO ₄	9.77	338.1387	-3.5	323.1349,308.0919,307.0835	Alkaloids	E.H.Wilson	
						353.0891, 191.0576,		<i>Periploca forrestii</i> Schltr.	
45	Isochlorogenic acid a	C ₂₅ H ₂₄ O ₁₂	9.82	516.1268	3.5	179.0352	Organic acid		
						353.0891, 205.0482,		<i>Periploca forrestii</i> Schltr.	
46	5-O-caffeoyl-3-O-sinapoylquinic acid	C ₂₇ H ₂₈ O ₁₃	10.01	560.1529	-0.4	191.0576	Phenylpropanoids		
						353.0891, 191.0576,		<i>Periploca forrestii</i> Schltr.	
47	3-O-caffeoyl-4-O-sinapoylquinic acid	C ₂₇ H ₂₈ O ₁₃	10.13	560.1529	-0.4	179.0352	Phenylpropanoids		
						285.0415, 255.0303,		<i>Lysimachia paridiformis</i> var. <i>stenophylla</i> Franch.	
48	Afzelin	C ₂₁ H ₂₀ O ₁₀	10.37	432.1057	-2.1	227.0336	Flavonoid		
						663.231, 641.2882, 517.1687,		<i>Lysimachia paridiformis</i> var. <i>stenophylla</i> Franch.	
49	8-prenylkaempferol-3-O-rutinosyl-7-O-glucoside	C ₃₈ H ₄₈ O ₂₀	10.5	824.2739	2.7	355.1163, 299.0544	Flavonoid		
						517.1687, 355.1163,		<i>Lysimachia paridiformis</i> var. <i>stenophylla</i> Franch.	
50	8-prenylkaempferol-3,7-di-glucosid	C ₃₂ H ₃₈ O ₁₆	10.54	678.216	0.1		Flavonoid		

	e					299.0544		
51	8-prenylkaempferol-3-O-rutinoside	C ₃₂ H ₃₈ O ₁₅	10.9	662.2211	3.2	517.1687, 355.1163, 299.0544	Flavonoid	<i>Lysimachia paridiformis</i> var. <i>stenophylla</i> Franch.
52	4-O-caffeoyl-5-O-sinapoylquinic acid	C ₂₇ H ₂₈ O ₁₃	10.99	560.1529	-0.4	353.0891, 191.0576, 179.0352	Phenylpropanoids	<i>Periploca forrestii</i> Schltr.
53	N-feruloyltyramine	C ₁₈ H ₁₉ NO ₄	11.15	313.1314	1.9	297.1022, 190.0511	Alkaloids	<i>Sinomenium acutum</i> (Thunb.) Rehder & E.H.Wilson
54	Quercetin-3-O-(2"-p-coumaroyl)-β-d-glucoside	C ₃₀ H ₂₆ O ₁₄	11.22	610.1323	-3.1	463.0885, 301.04	Flavonoid	<i>Lysimachia paridiformis</i> var. <i>stenophylla</i> Franch.
55	Kaempferol-3-O-(2"-p-coumaroyl)-β-d-glucoside	C ₂₇ H ₃₀ O ₁₅	12.56	594.158	1	447.0932,285.0466	Flavonoid	<i>Lysimachia paridiformis</i> var. <i>stenophylla</i> Franch.
56	Periforoside e	C ₃₅ H ₅₂ O ₁₃	12.74	680.3409	0.1	517.2798	Glycoside	<i>Lysimachia paridiformis</i> var. <i>stenophylla</i> Franch.
57	Kaempferol-3-O-(3"-p-coumaroyl)-β-d-glucoside Periplogenin	C ₃₀ H ₂₆ O ₁₃	12.76	594.1373	-1.6	447.0976,285.0466	Flavonoid	<i>Lysimachia paridiformis</i> var. <i>stenophylla</i> Franch.
58	3-O-b-d-glucopyranosyl(1-4)-O-b-d-digitoxopyranoside	C ₃₅ H ₅₄ O ₁₃	12.93	682.3564	0.1	681.3502,519.2936	Steroid	<i>Periploca forrestii</i> Schltr.
59	Epimedin A	C ₃₉ H ₅₀ O ₂₀	13.02	838.2896	0.7	677.2479,531.1853,369.1335	Flavonoid	<i>Lysimachia paridiformis</i> var. <i>stenophylla</i> Franch.
60	Epimedin B	C ₃₈ H ₄₈ O ₁₉	13.22	808.279	4.9	677.2479,531.1853,369.1335	Flavonoid	<i>Lysimachia paridiformis</i> var. <i>stenophylla</i> Franch.
61	3b-[(O-b-d-glucopyranosyl(1-4)-b-d-cymarosyl)oxy]-5b, 14b-dihydroxy-7-en-card-20(22)-enolide	C ₃₆ H ₅₄ O ₁₃	13.24	694.3564	1	693.3514,531.2959	Glycoside	<i>Lysimachia paridiformis</i> var. <i>stenophylla</i> Franch.
62	Periplocin	C ₃₆ H ₅₆ O ₁₃	13.3	696.3721	3.2	695.3643,533.3135	Steroid	<i>Periploca forrestii</i> Schltr.
63	Epimedin C	C ₃₉ H ₅₀ O ₁₉	13.47	822.2946	-0.1	677.2479,531.1853,369.1335	Flavonoid	<i>Lysimachia paridiformis</i> var. <i>stenophylla</i> Franch.
64	Icariin	C ₃₅ H ₄₀ O ₁₅	13.6	676.2367	-2.8	531.1853,369.1335,313.0719	Flavonoid	<i>Lysimachia paridiformis</i> var. <i>stenophylla</i> Franch.
65	1,2-methylenedioxy-3,10,11-trimethoxynoraporphine	C ₂₀ H ₂₁ NO ₅	13.83	355.142	1.7	341.1246,326.1048,312.1241	Volatile oils	<i>Periploca forrestii</i> Schltr.
66	8-prenylkaempferol-3-O-glucosyl-7-O-rhamnoside	C ₃₂ H ₃₈ O ₁₅	15.39	662.2211	3.2	501.1796, 355.1163, 299.0544	Flavonoid	<i>Periploca forrestii</i> Schltr.
67	Canadine	C ₂₀ H ₂₁ NO ₄	15.81	339.1471	4.7	325.0968, 324.0867, 310.0741	Alkaloids	<i>Sinomenium acutum</i> (Thunb.) Rehder & E.H.Wilson
68	8-prenylkaempferol-3,7-di-O-rhamnoside	C ₃₂ H ₃₈ O ₁₄	16.04	646.2262	1.5	501.1796,355.1163,299.0544	Flavonoid	<i>Lysimachia paridiformis</i> var. <i>stenophylla</i> Franch.
69	Cannabisin F	C ₃₆ H ₃₆ N ₂ O ₈	16.12	624.2472	-2.1	462.1931,351.0867,325.1079	Organic acid	<i>Periploca forrestii</i> Schltr.
70	Cannabisin F isomer	C ₃₆ H ₃₆ N ₂ O ₈	16.3	624.2472	-2.1	462.1931,351.0867,325.1079	Organic acid	<i>Periploca forrestii</i> Schltr.
71	8-prenylkaempferol-3-O-rhamnoside e	C ₂₆ H ₂₈ O ₁₀	16.42	500.1682	-2.2	355.1163,299.0544	Flavonoid	<i>Lysimachia paridiformis</i> var. <i>stenophylla</i> Franch.
72	Chelidonine	C ₂₀ H ₁₉ NO ₅	18.06	353.1263	-1.1	339.1095,176.0717	Alkaloids	<i>Sinomenium acutum</i> (Thunb.) Rehder & E.H.Wilson
73	Icaritin-3-O-rutinoside	C ₃₃ H ₄₀ O ₁₅	18.65	676.2367	-2.8	531.1853,369.1335,313.0719	Flavonoid	<i>Lysimachia paridiformis</i> var. <i>stenophylla</i> Franch.
74	Nandazurine	C ₁₉ H ₁₄ NO ₅	19.66	336.0872	-1.5	318.0773,290.0817,262.0887	Alkaloids	<i>Sinomenium acutum</i> (Thunb.) Rehder & E.H.Wilson
75	Icaritin-3,7-O-di-rhamnoside	C ₃₃ H ₄₀ O ₁₄	20.11	660.2418	2.3	515.1929,369.1335,313.0719	Flavonoid	<i>Lysimachia paridiformis</i> var. <i>stenophylla</i> Franch.
76	Icaritin-3-O-rhamnoside	C ₂₁ H ₂₀ O ₆	21.62	514.1839	2.3	369.1335,313.0719	Flavonoid	<i>Lysimachia paridiformis</i> var. <i>stenophylla</i> Franch.

77	8-oxoepiberberine	C ₂₀ H ₁₇ NO ₅	24.87	351.1107	0.9	337.0966,322.0712,308.0919	Alkaloids	<i>Sinomenium acutum</i> (Thunb.) Rehder & E.H.Wilson
78	Α-linolenic acid	C ₁₈ H ₃₀ O ₂	28	278.2246	-2.9	/	Volatile oils	<i>Periploca forrestii</i> Schltr.
79	Linoleic acid	C ₁₈ H ₃₂ O ₂	28.57	280.2402	-3.6	/	Volatile oils	<i>Periploca forrestii</i> Schltr.
