

Supplementary information for

“Differentiation of *Lepidium meyenii* (Maca) from Different Origins by Electrospray Ionization Mass Spectrometry with Principal Component Analysis”

by

Sihou Yang, Xiaochun Sun, Yumei Gao, Rui Chen*

College of Chemistry and Chemical Engineering, Yunnan Normal University, Kunming 650500, China

Table S1 The information of chemical components in Maca extract

Sample Name	Formula	Ion type	Theoretical m/z	Detected m/z	Relative error (ppm)	MS/MS fragments
Benzyl nitrile	C ₇ H ₅ N	[M+H] ⁺	104.0500	104.0496	-3.8	91, 77, 58
Proline	C ₅ H ₉ NO ₂	[M+H] ⁺	116.0711	116.0706	-4.3	98, 85, 70
Arginine	C ₆ H ₁₄ N ₄ O ₂	[M+H] ⁺	175.1195	175.1190	-2.9	158, 129, 58
N-benzyl octanamide	C ₁₅ H ₂₃ NO	[M+H ₂ O+H] ⁺	252.1964	252.1969	2.0	155, 126, 109, 91
		[M+2H ₂ O+H] ⁺	270.2069	270.2074	1.9	
Lepidiline A	C ₁₉ H ₂₁ N ₂ Cl	[M-Cl] ⁺	277.1705	277.1709	1.4	185, 91, 59, 29
Lepidiline B	C ₂₀ H ₂₃ N ₂ Cl	[M-Cl] ⁺	291.1861	291.1855	-2.1	200, 199, 91, 29
N-benzyl hexadecanamide	C ₂₃ H ₃₉ NO	[M+H] ⁺	346.3110	346.3104	-1.7	268, 239, 221, 109, 91
N-benzyl-(9Z, 12Z)-octadecadienamide	C ₂₅ H ₃₉ NO	[M+H] ⁺	370.3110	370.3104	-1.6	263, 245, 109, 91
		[M+K] ⁺	408.2668	408.2663	-1.2	
sucrose	C ₁₂ H ₂₂ O ₁₁	[M+K] ⁺	381.0799	381.0794	-1.3	343, 325, 307, 289, 271
N-benzyl-5-oxo-6E, 8E-octadecadienamide	C ₂₅ H ₃₇ NO ₂	[M+H] ⁺	384.2903	384.2897	-1.6	277, 260, 108, 91
2-hydroxysuccinic acid	C ₄ H ₆ O ₅	[M-H] ⁻	133.0137	133.0142	3.8	117
D-allose	C ₆ H ₁₂ O ₆	[M-H] ⁻	179.0556	179.0561	2.8	161, 143, 125
palmitic acid	C ₁₆ H ₃₂ O ₂	[M-H] ⁻	255.2324	255.2330	2.4	225
linoleic acid	C ₁₈ H ₃₂ O ₂	[M-H] ⁻	279.2324	279.2320	-1.4	263

sucrose	C ₁₂ H ₂₂ O ₁₁	[M-H] ⁻	341.1084	341.1090	1.8	323, 305, 287, 269, 179, 161
3-hydroxypropyl glucosinolate	C ₁₀ H ₁₉ NO ₁₀ S ₂	[M-H] ⁻	376.0372	376.0366	-1.6	296, 275, 259, 241, 180, 134
benzyl glucosinolate	C ₁₄ H ₁₉ NO ₉ S ₂	[M-H] ⁻	408.0423	408.0428	-1.5	328, 275, 259, 241, 212, 166
ergocalciferol	C ₂₈ H ₄₄ O	[M+Cl] ⁻	431.3081	431.3086	1.2	395, 378
m-methoxybenzyl glucosinolate	C ₁₅ H ₂₁ NO ₁₀ S ₂	[M+H ₂ O-H] ⁻	456.0634	456.0629	-1.1	358, 275, 259, 241, 242, 196
		[M+2H ₂ O-H] ⁻	474.0740	474.0735	-1.1	
tetrasaccharide	C ₂₄ H ₄₂ O ₂₁	[M+H ₂ O-H] ⁻	683.2246	683.2241	-0.7	647, 629, 611, 593, 575, 557

Table S2 Comprehensive scores and ranks of the ingredients of Maca in positive mass spectra

Sample	PC1	PC2	PC3	PC4	Comprehensive score	Rank
Lijiang 2	-0.0275	0.2793	1.1539	1.4207	0.4266	1
Shangri-La 1	-0.2384	1.7932	-0.5089	-0.3423	0.3755	2
Peru 1	1.3719	0.0031	-0.4561	-1.2869	0.3247	3
Peru 3	0.5065	-0.1638	0.8968	0.1830	0.3054	4
Peru 2	-0.0460	-0.0084	0.4480	0.4910	0.1058	5
Shangri-La 3	0.1356	-0.1680	-0.5573	0.9744	0.0345	6
Shangri-La 2	-0.0177	-0.1892	-0.5511	1.3615	0.0144	7
Lijiang 3	-0.0674	-0.1667	1.2277	-1.0840	-0.0302	8
Lijiang 1	0.1073	-0.3977	-0.9980	0.7214	-0.1490	9
Huize 2	-0.5974	-0.2103	0.4557	-0.7595	-0.3325	10
Huize 3	-0.5417	-0.2910	-0.4525	-0.9715	-0.4985	11
Huize 1	-0.5851	-0.4805	-0.6582	-0.7080	-0.5767	12

Table S3 Comprehensive scores and ranks of the ingredients of Maca in negative mass spectra

Sample	PC1	PC2	PC3	PC4	Comprehensive score	Rank
Peru 2	-0.1870	0.0233	2.1294	0.1296	0.4218	1
Shangri-La 2	0.61636	0.3865	0.7715	-0.5944	0.3412	2
Huize 3	-0.2736	1.1152	-0.3698	0.3136	0.1985	3
Huize 1	0.4123	0.4592	-0.32164	-0.1835	0.1492	4
Huize 2	-0.5035	0.9258	-0.5769	0.7980	0.1295	5
Lijiang 1	0.3948	-1.2600	0.0041	1.4452	0.0816	6
Lijiang 2	-0.1823	-0.2170	-0.3455	0.8947	-0.0070	7
Peru 1	0.6639	-0.0025	-0.4756	-0.6055	-0.0132	8
Shangri-La 3	-0.5749	0.1211	0.2949	0.1332	-0.0608	9
Shangri-La 1	0.6486	-0.1083	-0.2117	-0.9659	-0.0641	10
Peru 3	0.3821	-0.6007	-0.58114	-0.1435	-0.1916	11
Lijiang 3	-1.39687	-0.8426	-0.3177	-1.2215	-0.9850	12