Supplementary Material

UPLC-Q-Orbitrap-MS/MS for Rapid Characterization of the Chemical Constituents of *Atractylodis lancea* and *Atractylodis macrocephalae*

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Table S1: Details of the identified peaks, such as retention times, molecular formulas, ion types, detected masses, mass errors, fragment ions, and sources.

No.	Compound	T_R(min)	Molecular formula	Detected mass (*m/z*)	Ion type	Mass error (ppm)	MS/MS (*m/z*)	Source
1	Caryophyllene oxide	9.919	C15 H24 O	221.18964	[M+H]+1	-3.88	203.17807, 147.11588, 133.10028, 95.08492	Cangzhu, Baizhu
2	Turmerone	5.333	C15 H20 O	217.15829	[M+H]+1	-4.17	199.14670, 175.14688, 161.09502, 107.08479	Cangzhu, Baizhu
3	Artemisinin	9.244	C15 H22 O5	283.15325	[M+H]+1	-4.43	237.14709, 219.13667, 191.14189	Baizhu
4	6,11-Dihydroxyeudesmane	13.078	C15 H28 O2	239.19993	[M-H]-1	-4.9	179.05524, 61.98806, 59.01357	Cangzhu
5	4α,8α-dihydroxyeudesman-11-en-1-one	9.792	C15 H24 O3	251.16349	[M-H]-1	-4.82	61.98804	Cangzhu
6	1α-hydroxy-1-desoxotamirin	8.039	C15 H20 O4	265.14308	[M+H]+1	-3.48	247.13148, 229.12100, 205.12114	Baizhu

7	10,11,12-Guaianetriol	3.497	C15 H28 O6 S	335.15136	[M-H]-1	-4.3	80.96479, 96.95966, 175.08691	Baizhu
8	Geraniol	8.744	C10 H18 O	153.12722	[M-H]-1	-4.45	99.08102, 97.06537	Cangzhu
9	(6S)-hydroxymenthol	10.576	C10 H20 O2	171.13779	[M-H]-1	-4.16	125.89182, 89.02396, 61.98806	Cangzhu
10	Camphor	5.874	C10 H16 O	153.12731	[M+H]+1	-3.87	135.11592, 109.10046, 43.05394	Cangzhu
11	Delta-4-Carene	12.111	C10 H16	135.11676	[M-H]-1	-4.74	117.91853, 7500841	Cangzhu
12	Aplotaxene	12.568	C17 H28	231.21045	[M-H]-1	-3.69	187.98769, 146.96519, 61.98805, 59.01354	Cangzhu
13	Rosiridin	5.701	C16 H28 O7	333.19031	[M+H]+1	-2.96	85.02778, 135.11592, 279.15726	Cangzhu
14	Furopinnarin	9.996	C17 H16 O4	285.11168	[M+H]+1	-3.59	165.06879, 225.08954	Cangzhu
15	7-hydroxy-6-methoxy-2H-chromen-2-one	4.251	C10 H8 O4	193.04954	[M+H]+1	-2.91	133.0275	Cangzhu, Baizhu
16	Marmesin	6.514	C14 H14 O4	247.09588	[M+H]+1	-4.55	229.08438, 201.08969	Cangzhu
17	5,6-dimethoxy-2-(2-methoxyphenyl)-4H-chromen-4-one	7.109	C18 H16 O5	313.10904	[M+H]+1	4.61	185.13129	Baizhu
18	Psoracorylifol C	12.259	C18 H24 O3	287.16333	[M-H]-1	-4.78	61.98812, 79.95704, 243.17433	Baizhu
19	Iristectorin B	6.669	C23 H24 O12	493.13276	[M+H]+1	-3.74	331.07892, 85.02783	Cangzhu
20	Quercetol B	12.324	C23 H28 O4	367.18981	[M-H]-1	-2.98	279.21060, 308.17679, 323.20023	Baizhu
21	4-Methoxycinnamaldehyde	6.272	C10 H10 O2	163.07538	[M+H]+1	-3.2	131.04823, 103.05423	Cangzhu, Baizhu
22	4-methoxy-6-(prop-2-en-1-yl)-2H-1,3-benzodioxole	8.789	C11 H12 O3	193.08560	[M+H]+1	-4.68	133.064	Cangzhu
23	3-hydroxy-2,5-toluquinone	3.785	C7 H6 O3	137.02322	[M-H]-1	-4.97	93.03407	Cangzhu
24	Coniferyl aldehyde	4.511	C10 H10 O3	177.05433	[M-H]-1	-4.93	162.03146,133.02888,105.03410	Cangzhu
25	Arginine	0.676	C6 H14 N4 O2	175.11894	[M+H]+1	-3.17	116.06982, 60.05523	Cangzhu, Baizhu
26	Isoleucine	1.19	C6 H13 N O2	132.10216	[M+H]+1	-2.61	86.09586, 87.09922	Cangzhu
27	Phenylalanine	2.088	C9 H11 N O2	164.07051	[M-H]-1	-4.21	148.06036, 147.04437, 72.00871	Cangzhu
28	Ornithine	0.671	C5 H12 N2 O2	131.08146	[M-H]-1	-4.9	115.92013, 85.07668, 59.01357	Cangzhu
29	Tyrosine	1.059	C9 H11 N O3	180.06554	[M-H]-1	-3.12	163.03925, 119.04963, 72.00873	Cangzhu, Baizhu

30	Alanine	0.686	C3 H7 N O2	88.03949	[M-H]-1	-4.67	71.01350, 59.01355	Cangzhu, Baizhu
31	Asparagine	0.684	C4 H8 N2 O3	131.04506	[M-H]-1	-4.87	115.92013, 85.07668, 59.01357	Cangzhu
32	Aspartic acid	0.753	C4 H7 N O4	134.04494	[M+H]+1	-2.68	87.05478	Baizhu
33	Tryptophan	3.143	C11 H12 N2 O2	203.08126	[M-H]-1	-4.14	72.00875, 116.05000, 159.09200	Baizhu
34	Phenylalaninamide	2.457	C9 H12 N2 O	163.08634	[M-H]-1	-4.63	72.00876, 107.06101, 147.04448	Baizhu
35	N-Acetyl-L-isoleucine	5.321	C8 H15 N O3	172.09667	[M-H]-1	-4.24	58.02957, 128.10751, 130.08673	Baizhu
36	N-Acetyl-L-leucine	5.521	C8 H15 N O3	172.09673	[M-H]-1	-3.88	58.02954, 79.95698, 130.08673	Baizhu
37	Isovalerylglycine	5.107	C7 H13 N O3	158.08105	[M-H]-1	-4.13	79.95698, 114.09189, 130,08675	Baizhu
38	guanidinoacetate	4.146	C3 H6 N3 O2	115.08361	[M-H]-1	3.58	85.02908, 71.01348, 68.99540	Cangzhu
39	L-Pyroglutaminol	0.733	C5 H9 N O2	114.05514	[M-H]-1	-3.13	85.02909, 71.01349, 66.03458	Cangzhu
40	Tryptamine	3.132	C10 H12 N2	159.09156	[M-H]-1	-4.04	129.01866, 116.92796, 116.07113	Cangzhu
41	Suberylglycine	5.304	C10 H17 N O5	230.10183	[M-H]-1	-4.21	79.95700, 98.02431, 168.10222	Baizhu
42	Acetylcarnitine	5.475	C9 H17 N O4	202.10709	[M-H]-1	-3.99	59.01356, 79.95698, 130.08672, 158.11789	Baizhu
43	Linoleic acid	13.560	C18 H32 O2	279.23155	[M-H]-1	-3.06	261.22137, 127.66266, 59.01355	Cangzhu, Baizhu
44	Lauric acid	12.119	C12 H24 O2	199.16799	[M-H]-1	-4.99	152.91064, 106.91794, 61.98804	Cangzhu
45	Aseanostatin P1	13.068	C14 H28 O2	227.19999	[M-H]-1	-4.88	183.13824, 165.12776, 61.98809	Cangzhu
46	Aseanostatin P5	13.377	C15 H30 O2	241.21561	[M-H]-1	-4.95	212.91866, 148.91551, 118.91766, 61.98806	Cangzhu
47	Margaric acid	14.205	C17 H34 O2	268.24754	[M-H]-1	-2.08	225.18494, 130.94356, 117.65070	Cangzhu
48	2-decenoicacid	10.092	C10 H18 O2	169.12213	[M-H]-1	-4.58	151.11215, 122.89355	Cangzhu
49	Caprylic acid	9.374	C8 H16 O2	143.10654	[M-H]-1	-4.59	61.98803	Cangzhu
50	Margaric acid	14.112	C17 H34 O2	269.24729	[M-H]-1	-3.02	225.18452, 207.17445	Cangzhu
51	Dodecenoic acid	11.859	C12 H22 O2	197.15360	[M-H]-1	-3.04	103.97601, 61.98804	Cangzhu
52	7-Tetradecenoic acid	12.48	C14 H26 O2	225.18441	[M-H]-1	-4.86	61.98804	Cangzhu
53	(E)-2-decenoicacid	9.26	C10 H18 O2	169.12215	[M-H]-1	-4.46	122.89355, 96.95959, 68.99539	Cangzhu
54	12-Hydroxyoctadecanoic acid	13.549	C18 H36 O3	299.25756	[M-H]-1	-3.47	59.01357	Cangzhu
55	11-methyldodecanoic acid	12.48	C13 H26 O2	213.18449	[M-H]-1	-4.75	185.89980, 167.88934, 121.89670, 61.98805	Cangzhu
56	11-methyldodecanoic acid	12.613	C13 H26 O2	213.18447	[M-H]-1	-4.81	185.89981, 61.98805	Cangzhu

57	Arachidonic acid	13.453	C20 H32 O2	303.23091	[M-H]-1	-4.93	259.24176, 59.01355	Cangzhu
58	Dehydromatricarianol	9.411	C10 H8 O	143.04906	[M-H]-1	-4.49	61.98803	Cangzhu
59	2,4,6,8,10,12-tetradeca-1,14-hexenedial	9.823	C14 H14 O2	213.09065	[M-H]-1	-4.44	185.89984, 167.88939, 61.98807	Cangzhu
60	2,3-Dihydroxydodecanoate	10.203	C12 H23 O4	232.16857	[M+H]+1	4.61	196.15215	Baizhu
61	8-Hydroxydodecanoate	7.275	C12 H23 O3	216.17321	[M+H]+1	3.27	198.17331	Baizhu
62	Glutaral	1.801	C5 H8 O2	99.04418	[M-H]-1	-4.23	58.00573, 67.01861, 80.96291	Baizhu
63	8-hydroxyjasmonic acid	7.846	C12 H18 O4	225.11170	[M-H]-1	-4.44	181.12244, 61.98804	Cangzhu, Baizhu
64	12-hydroxyjasmonic acid	7.85	C12 H18 O4	225.11199	[M-H]-1	-3.16	61.98808, 163.11206, 181.12256	Baizhu
65	Pentadecanoic acid	13.471	C15 H30 O2	241.21578	[M-H]-1	-4.21	61.98809, 118.91769, 212.91872	Baizhu
66	3-Hydroxymyristic Acid	11.815	C14 H28 O3	243.19548	[M-H]-1	-2.13	59.01358, 61.98809, 197.90555	Baizhu
67	Methyl oleate	14.359	C19 H36 O2	295.26249	[M-H]-1	-4.11	87.00838, 98.95541, 217.87003	Baizhu
68	13-Eicosenoic acid	14.708	C20 H38 O2	309.27786	[M-H]-1	-4.97	115.92029, 130.94366, 221.14353	Baizhu
69	Mesaconic acid	0.973	C5 H6 O4	129.01819	[M-H]-1	-4.71	101.02389, 85.02906	Cangzhu
70	Lactic acid	0.929	C3 H6 O3	89.02347	[M-H]-1	-4.84	71.01348, 59.01353	Cangzhu, Baizhu
71	Aminocaproic acid	1.203	C6 H13 N O2	130.08616	[M-H]-1	-4.89	88.03993	Cangzhu, Baizhu
72	Neuraminic acid	1.871	C9 H17 N O8	268.10271	[M+H]+1	-1.83	136.06087	Cangzhu, Baizhu
73	Cis-cascarillic acid	10.409	C11 H20 O2	183.13764	[M-H]-1	-4.69	59.01359, 109.02904, 122.98382	Baizhu
74	Isopentyl cinnamate	9.085	C14 H18 O2	217.12222	[M-H]-1	-3.15	59.01357, 174.99167, 189.00782	Baizhu
75	Uracil	1.083	C4 H4 N2 O2	113.03473	[M+H]+1	-3.31	113.03374	Cangzhu
76	2'-O-Methylguanosine 5'-monophosphate	6.223	C11 H16 N5 O8 P	376.06497	[M-H]-1	-2.22	269.08044, 61.98801	Cangzhu
77	N-Methoxy-2-nitroadenosine	3.717	C11 H14 N6 O7	341.08561	[M-H]-1	2.95	179.03397, 89.02392	Cangzhu
78	5-carboxycytosine	0.694	C5 H5 N3 O3	156.04158	[M+H]+1	4.35	110.0706	Baizhu
79	Thymidine	2.237	C10 H14 N2 O5	241.08127	[M-H]-1	-4.7	59.01355, 75.00841, 135.05573, 196.10817	Baizhu

80	Guanosine	1.411	C10 H13 N5 O5	282.08243	[M-H]-1	-4.85	80.96481, 133.01494, 150.04138	Baizhu
81	4-Vinylresorcinol	4.725	C8 H8 O2	135.04394	[M-H]-1	-4.92	116.00645, 107.04967, 91.01840	Cangzhu
82	2,4-Di-t-butylphenol	11.531	C14 H22 O	205.15818	[M-H]-1	-4.95	61.98804	Cangzhu
83	Methyl caffeate	4.465	C10 H10 O4	195.06503	[M+H]+1	-3.45	135.04314, 161.05859, 167.06911	Cangzhu
84	Resorcinol	2.916	C6 H6 O2	109.02846	[M-H]-1	-4.99	95.01335, 85.02902, 81.03418, 66.03455	Cangzhu
85	Phenol	5.86	C6 H6 O	93.03357	[M-H]-1	-4.57	81.70591, 61.58095	Cangzhu, Baizhu
86	Lapachol	8.961	C15 H14 O3	243.10144	[M+H]+1	-2.73	226.17871, 200.08194	Cangzhu
87	9-methylparagracine	10.697	C14 H18 N6	271.16798	[M+H]+1	3.25	103.05355, 137.05881, 211.11031	Cangzhu
88	Atropine	8.824	C17 H23 N O3	290.17456	[M+H]+1	-3.57	244.16797,231.13638, 213.12598	Baizhu
89	Bohemamine	5.106	C14 H18 N2 O3	261.12280	[M-H]-1	-4.21	94.98042, 141.06630, 155.08189	Baizhu
90	Roquefortine C	9.824	C22 H23 N5 O2	388.17558	[M-H]-1	-4.44	96.95967, 138.01904, 249.14845	Baizhu
91	N-methyl-γ-oxo-3-Pyridinebutanamide	2.45	C10 H12 N2 O2	191.08118	[M-H]-1	-4.79	87.00835, 111.00822, 163.08691	Baizhu
92	Laudanosine	8.939	C21 H27 N O4	358.20068	[M+H]+1	-3.12	342.16271, 298.17831, 84.08028	Baizhu
93	Glycyl-L-leucyl-L-prolyl-L-α-glutamylglycylglycine	6.654	C22 H36 N6 O9	529.26182	[M+H]+1	-0.72	161.09499, 217.15720, 397.21954	Cangzhu
94	Gly-Asp	0.651	C6 H10 N2 O5	189.05021	[M-H]-1	-4.7	74.02439, 96.00864, 114.01909	Baizhu
95	γ-L-glutamyl-L-leucine	4.063	C11 H20 N2 O5	259.12829	[M-H]-1	-4.29	128.03470, 197.12860, 241.11824	Baizhu
96	Pro-Ser	5.474	C8 H14 N2 O4	201.08669	[M-H]-1	-4.03	80.96480, 127.05069, 185.05586	Baizhu
97	2,3,4-Trihydroxybutanamide	1.877	C4 H9 N O4	136.06144	[M+H]+1	3.21	43.01755	Cangzhu
98	Damascenone	12.11	C13 H18 O	189.12696	[M-H]-1	-4.95	97.06538, 83.04982, 61.98804, 57.03428	Cangzhu
99	Benzoic acid	6.405	C7 H6 O2	121.02847	[M-H]-1	-4.35	61.98805, 93.03410, 108.02110	Baizhu
100	Cannabidivarin	12.76	C19 H26 O2	287.19997	[M+H]+1	-3.92	229.15732	Baizhu
101	O-(α-D-mannosyl)-L-threonine	2.981	C10 H19 N O8	282.11836	[M+H]+1	-1.9	136.06091, 137.05791	Baizhu
102	Hexitol	0.706	C6 H14 O6	181.07029	[M-H]-1	-5.01	80.96481, 138.05539, 163.03929	Baizhu
103	1,5-anhydroxylitol	1.605	C5 H10 O4	133.04949	[M-H]-1	-4.57	71.01351, 89.02400, 115.00311	Baizhu
104	L-Threose	5.26	C4 H8 O4	119.03393	[M-H]-1	-3.99	43.01864, 59.01355, 101.02394	Baizhu
105	Farinomalein	4.84	C10 H13 N O4	210.07572	[M-H]-1	-4.2	61.98807, 79.95698, 96.95964, 124.03979	Baizhu

106	Maniwamycin A	4.827	C10 H18 N2 O2	197.12815	[M-H]-1	-4.32	79.95699, 109.01643, 120.99583	Baizhu
107	Pseudopyronine B	11.3	C17 H30 O3	281.21032	[M-H]-1	-4.9	79.95701, 87.00838, 219.13806	Baizhu
108	Mucidone	6.636	C11 H16 O2	179.10643	[M-H]-1	-4.32	87.00836, 96.96916, 161.04480	Baizhu
109	Muscone	14.167	C16 H30 O	239.23654	[M+H]+1	-4.01	57.06955, 95.08498	Baizhu
110	Sistodiolynne	2.072	C9 H8 O2	147.04390	[M-H]-1	-4.75	72.99277, 75.00844, 115.00314	Baizhu
111	Pantothenic acid	2.881	C9 H17 N O5	218.10185	[M-H]-1	-4.35	59.01357, 88.03997, 146.08157	Cangzhu, Baizhu