

Supplementary Table S2. liquid chromatography electrospray ionisation tandem mass spectrometry (LC-ESI-MS/MS) analysis of Andrographis paniculate leaf.

	Molecular mass (calculated)	Mass spectrum (m/z) fragment ion (positive mode)	Retention time (min)	Formular	Identified compounds	KS	UT	CR	CM	RB
1	522.5016	540.5355	35.408	C ₃₄ H ₆₆ O ₃	Tetrahydro-6-(2-hydroxy-16,19-dimethylhexacosyl)-4-methyl-2H-pyran-2-one	0.28	0	0	0	0
2	475.6175	452	33.42	C ₂₇ H ₄₁ NO ₆	Hydrocortamate	0	0.04	0	0	0
3	281.272	282.28	34.377	C ₁₈ H ₃₅ N O	Dodemorph	0	0	0	4.78	0
4	384.3237	402.3575	26.067	C ₂₃ H ₄₄ O ₄	MG(0:0/20:1(11Z)/0:0)	0	0.04	0	0	0
5	604.9	137.4376	21.87	C ₃₈ H ₆₈ O ₅	DG(15:0/20:3(5Z,8Z,11Z)/0:0)	0.01	0	0	0	0
6	255.2568	256.2641	33.587	C ₁₆ H ₃₃ N O	Palmitic amide	0	0	0	1.23	0
7	429.43	319.43	20.08	C ₃₇ H ₆₄ O ₄	Dieporeticenin	0	0	0	0.05	0
8	572.9	407.22	23.557	C ₁₈ H ₃₄ N ₂ O ₆ S	Lincomycin	0	0.05	0	0	0
9	661.9	453.54	34.5	C ₃₆ H ₆₃ N ₅ O ₆	Cer(d18:0/12:0)	0	0	0	0	0.02
10	484.2829	507.272	32.009	C ₂₉ H ₄₀ O ₆	Stigmatellin Y	0	0	0	0.04	0
11	512.3142	530.3479	31.976	C ₃₁ H ₄₄ O ₆	Carindone	0	0	0	0.02	0
12	459.2628	460.2701	21.176	C ₂₆ H ₃₇ N O ₆	Militarinone A	0	0.02	0	0	0
13	370.7	453.75	31.8	C ₂₇ H ₄₆	Cholest-5-ene	0	0	0	0.05	0
14	301.298	302.3053	22.409	C ₁₈ H ₃₉ N O ₂	Sphinganine	0	0.17	0	0	0
15	306.1841	324.2178	26.577	C ₁₉ H ₂₂ N ₄	Corrinoid	0.03	0	0	0	0
16	268.2767	286.3105	22.386	C ₁₈ H ₃₆ O	Oleyl alcohol	0	0.15	0	0	0
17	225.28	245.48	22.32	C ₁₅ H ₁₅ NO	Navenone A	0	0.07	0	0	0
18	407.4	359.54	18.52	C ₁₉ H ₂₁ NO ₇ S	Erysothiopine	0	0.02	0	0	0
19	305.2355	306.2428	25.47	C ₁₉ H ₃₁ N O ₂	Samandarine	0	0	0	0.05	0
20	386.1725	409.1617	21.692	C ₂₂ H ₂₆ O ₆	Porson	0	0.17	0	0	0
21	196.219	214.2528	21.319	C ₁₄ H ₂₈	Cyclotetradecane	0	0.49	0	0	0

22	312.5304	484.1341	12.98	C ₂₀ H ₄₀ O ₂	3L,7D,11D-phytanic acid	0	0	0	0	0.04
23	469.3036	492.2931	23.351	C ₂₅ H ₄₃ N O ₇	Methymycin	0	0	0	0.11	0
24	542.03	162.1253	21.356	C ₂₁ H ₄₂ O ₄	Polyoxyethylene 40 monostearate	0	0	0	0	0.03
25	474.59	221.1778	24.925	C ₂₇ H ₃₈ O ₇	Lucidenic acid L	0.06	0	0	0	0
26	226.2299	244.2637	20.725	C ₁₅ H ₃₀ O	2-Pentadecanone	0.24	0.07	0.5	0.5	0.66
27	316.2627	334.2965	17.98	C ₁₈ H ₃₆ O ₄	MG(0:0/15:0/0:0)	0	0.11	0	0	0
28	284.235	302.2687	20.977	C ₁₇ H ₃₂ O ₃	Muricatacin	0	0	0	0.08	0
29	283.41	170.0134	20.835	C ₁₆ H ₂₉ NO ₃	(+/-)-N,N-Dimethyl menthyl succinamide	0	0	0	0	0.12
30	317.2935	318.30	20.293	C ₁₈ H ₃₉ N O ₃	Phytosphingosine	0	0	0	5.98	0
31	273.2668	274.27	20.122	C ₁₆ H ₃₅ N O ₂	C16 Sphinganine	0	0	0	0	15.68
32	298.1937	299.2009	19.805	C ₂₀ H ₂₆ O ₂	Juvocimene 2	0	0	0	0	0.06
33	488.6	405.3456	26.427	C ₂₄ H ₄₀ O ₈ S	7-Sulfocholic acid	0	0	0	0	0.04
34	286.1938	287.2011	19.804	C ₁₉ H ₂₆ O ₂	Citronellyl cinnamate	0	0	0	0	0.07
35	258.1624	259.1697	19.805	C ₁₇ H ₂₂ O ₂	Cicutoxin	0	0	0	0	0.08
36	372.6	273.2669	19.687	C ₂₁ H ₂₈ N ₂ S ₂	Buthiobate	0	0	0	0	0.03
37	309.3042	310.3115	34.904	C ₂₀ H ₃₉ N O	N-Hexadecanoylpyrrolidine	0	0	0.53	0	0
38	368.2915	369.2986	33.187	C ₂₂ H ₄₀ O ₄	Octadecyl fumarate	0	0	0.03	0	0
39		212.21	30.112		Xylostasin	0	0.09	0.08	3.48	0
40	537.9	225.1148	19.329	C ₃₄ H ₆₇ NO ₃	N-Palmitoylsphingosine	0	0	0.04	0	0
41	387.25	282.28	31.986	C ₁₈ H ₃₅ N O	Oleamide	0	0	5.29	0	0
42	405.6	406.2127	26.75	C ₂₂ H ₄₇ NO ₅	Aminopentol	0.16	0.06	0.13	0.13	0.36
43	262.2307	280.26	29.872	C ₁₈ H ₃₀ O	6,10,14-Trimethyl-5,9,13-pentadecatrien-2-one	0	2.1	1.74	1.74	1.63
44	428.3123	429.3197	29.215	C ₂₄ H ₄₄ O ₆	Sorbitan oleate	0	0	0.05	0	0
45	402.2268	425.2161	28.919	C ₂₁ H ₃₀ N ₄ O ₄	Cinitapride	0	0	0.07	0	0
46	588.6	398.2442	30.566	C ₃₁ H ₄₀ O ₁₁	Sandoricin	0	0.05	0	0	0
47	576.7	281.272	32.955	C ₃₆ H ₃₆ N ₂ O ₅	Tiliacorine	0	0	0	0.04	0
48	398.2459	421.2353	25.982	C ₂₅ H ₃₄ O ₄	Pregna-5,16,20-triene-3beta,20-diol diacetate	0	0	0.03	0	0
49	272.42	268.2765	36.057	HO(CH ₂) ₁₅ CO ₂ H	16-hydroxy hexadecanoic acid	0	0.11	0	0.17	0.15
50	398.2445	421.2338	25.554	C ₁₈ H ₃₉ O ₇ P	Tris(butoxyethyl)phosphate	0	0	0.04	0	0

51	448.2813	449.2887	25.503	C ₂₆ H ₄₀ O ₆	(ent-2b,4S,9a)-2,4,9-Trihydroxy-10(14)-oplopen-3-one 2-(2-methylbutanoate) 9-(3-methyl-2E-pentenoate)	0	0	0.02	0	0
52	428.5	226.23	25.301	C ₂₄ H ₂₈ O ₇	1-Isomangostin hydrate	0	0.04	0	0	0
53	294.53	414.2041	9.27	C ₈ H ₁₆ N ₂ O ₃ S	Alanyl-Methionine	0	0.04	0	0	0
54	783.27	384.324	13.997	C ₁₆ H ₂₈ O ₁₃	b-D-Xylopyranosyl-(1->4)-a-L-rhamnopyranosyl-(1->2)-D-fucose	0.01	0	0	0	0
55	428.39	275.1484	4.421	C ₂₄ H ₄₂ O ₇ P ₂	SR 12813	0	0	0	0	0.09
56	270.4	356.2331	15.734	C ₁₈ H ₂₂ O ₂	3-Hydroxyestra-1,3,5(10)-trien-16-one	0.02	0.13	0	0	0.04
57	332.4	278.1518	9.276	C ₂₀ H ₂₈ O ₄	13-Hydroxy-2-(hydroxymethylene)-3-oxo-13,17-seco-5alpha-androstan-17-oic acid, delta-lactone	0	0	0	0	0.16
58	332.4	640.325	15.734	C ₁₄ H ₂₃ NO	N-Isobutyl-2,4,8-decatrienamide	0	0	0	0	0.05
59	1103.2	296.1776	16.659	C ₅₄ H ₈₆ O ₂₃	Protoprimulagenin A 3-[rhamnosyl-(1->4)-rhamnosyl-(1->4)-[rhamnosyl-(1->2)]-glucosyl-(1->?)-glucuronide]	0	0	0	0.02	0
60	502.2583	503.2657	15.767	C ₂₈ H ₃₈ O ₈	Cavipetin B	0.17	0	0	0	0
61	414.2058	432.2397	19.079	C ₂₄ H ₃₀ O ₆	Armillaripin	0.22	1.04	0.23	0	0.22
62	182.204	200.2379	18.505	C ₁₃ H ₂₆	1-Tridecene	0.08	0.09	0.14	0.14	0.21
63	182.0706	205.06	12.665	C ₆ H ₁₅ O ₄ P	Triethyl phosphate	0	0	0	0	5.18
64	154.0393	155.0468	12.688	C ₄ H ₁₁ O ₄ P	Diethylphosphate	0	0	0	0	0.13
65	300.4351	300.20893	18.092	C ₂₀ H ₂₈ O ₂	17alpha-Methyl-17beta-hydroxyandrosta-4,6-dien-3-one	0.03	0	0	0	0
66	318.4	405.3456	19.813	C ₂₀ H ₃₀ O ₃	4,5alpha-Dihydro-2-(hydroxymethylene)testosterone	0.21	0.04	0.17	0.17	0.1
67	463.32	453.3091	20.801		I-123 BMIPP	0.04	0	0	0	0
68	334.2153	357.2046	17.268	C ₂₀ H ₃₀ O ₄	6Î²,7Î²-Dihydroxykaurenoic acid	0.15	0.12	0.21	0.25	0.16
69	446.0868	447.0941	11.411	C ₂₁ H ₁₈ O ₁₁	Glucorhein	0	0	0	0.04	0
70	564.2283	565.2353	15.784	C ₂₂ H ₃₆ N ₄ O ₁₃	Aerobactin	0	0	0.07	0	0
71	316.2047	317.212	17.209	C ₂₀ H ₂₈ O ₃	17beta-Hydroxy-17-methylandrosta-4-ene-3,11-dione	0.12	0.36	0.18	0.31	0.14
72		414.2041	21.356	C ₂₀ H ₃₀ O ₅	15-dehydro-prostaglandin I2	0.02	0.04	0.34	0.34	0.24

73	446.4	316.204	14.544	C ₁₈ H ₂₂ O ₁₁ S	Paederoside	0	0.19	0	0	0
74	170.0142	188.0481	14.012	C ₈ H ₇ Cl O ₂	4-Chlorophenylacetic acid	0.06	0.11	0.13	0.13	0.17
75	518.5	386.1729	19.351	C ₂₀ H ₃₀ N ₄ O ₁₂	Poly-g-D-glutamate	0	0.08	0	0	0
76	448.12	373.1996	13.128	C ₂₀ H ₃₀ O ₅	Oryzalic acid B	0	0	0.03	0	0
77	496.2772	519.2662	13.572	C ₂₁ H ₃₆ N ₈ O ₆	APGPR Enterostatin	0	0	0.15	0	0
78	241.1468	242.1541	12.812	C ₁₆ H ₁₉ N O	Dehydroisochalciporone	0	0	0	0	0.19
79	296.4	262.23	30.69	C ₂₀ H ₂₄ O ₂	5-Methoxy-1,7-diphenyl-3-heptanone	0	0.03	0	0	0
80	404.183	405.1903	13.622	C ₂₂ H ₂₈ O ₇	Eupaserrin	0	0.06	0	0	0
81	162.126	185.1152	11.827	C ₈ H ₁₈ O ₃	(3R,7R)-1,3,7-Octanetriol	0.17	0.12	0.17	0.21	0.23
82	608.7	483.4652	18.884	C ₃₆ H ₃₆ N ₂ O ₇	Somniferine	0	0.07	0	0	0
83	757.4675	780.4572	10.719	C ₄₃ H ₆₈ N O ₈ P	PE(18:4(6Z,9Z,12Z,15Z)/20:5(5Z,8Z,11Z,14Z,17Z))	0	0	0.01	0	0
84	514.3084	537.2978	9.261	C ₃₄ H ₄₂ O ₄	Flavidulol C	0	0	0.03	0	0
85	399.4	555.523	16.893	C ₂₁ H ₁₉ F ₂ N ₃ O ₃	Difloxacin	0.01	0	0	0	0
86	293.1487	294.1559	3.745	C ₁₂ H ₂₃ N O ₇	N-(1-Deoxy-1-fructosyl)leucine	0	0	0.03	0	0
87	197.1205	198.1278	12.726	C ₁₄ H ₁₅ N	2-(3-Phenylpropyl)pyridine	0.25	0.11	0.43	0.62	0.6
88	386.1203	387.1277	3.739	C ₁₇ H ₂₂ O ₁₀	1-O-Sinapoylglucose	0	0	0.01	0	0
89	431.5	318.2194	6.55	C ₁₉ H ₃₇ N ₅ O ₆	Istamycin C1	0	0	0	0.05	0
90	330.34	278.1518	9.27	C ₁₆ H ₁₈ N ₄ O ₄	Pseudomonine	0.03	0	0	0	0
91	117.0789	140.0681	4.169	C ₅ H ₁₁ NO ₂	Norvaline	0	0	0.08	0	0
92	117.15	262.23	2.954	C ₅ H ₁₁ NO ₂	Isoamyl nitrite	0	0	0.45	0	0
93	590.71	350.2095	20.02	C ₃₆ H ₃₈ N ₄ O ₄	Dimethylprotoporphyrin IX dimethyl ester	0	0.39	0	0	0
94	406.5	226.1679	4.421	C ₂₅ H ₂₆ O ₅	Kanzonol Z	0.02	0	0	0	0
95	555.5237	578.5129	32.164	C ₃₄ H ₆₉ NO ₄	Armillaramide	0.07	0.02	0.05	0.02	0.09
96	226.1687	249.1579	5.306	C ₁₂ H ₂₂ N ₂ O ₂	1,8-Diazacyclotetradecane-2,9-dione	0.35	0	0.35	0.44	0.46
97	354.31	305.2353	22.371	C ₁₆ H ₁₈ O ₉	Cis-5-Caffeoylquinic acid	0	0.04	0	0	0
98	174.11	225.1148	19.07	C ₆ H ₆ O ₆	trans-Aconitate	0.02	0	0	0	0
99	208.21	168.1879	19.492	C ₈ H ₁₆ O ₆	Ethyl beta-D-glucopyranoside	0.06	0.19	0	0	0

100		278.1517	16.241	C ₇ H ₈ N ₄ O ₂	Theophylline	0.1	0	0	0	0
101	278.1529	301.1422	26.998	C ₁₆ H ₂₂ O ₄	Alpha-CEHC	0.26	0.1	0.26	0.27	0.31
102	382.5	86.0734	15.734	C ₂₂ H ₃₈ O ₅	Misoprostol	0	0.01	0	0	0
103	342.3	166.06	13.999	C ₁₂ H ₂₂ O ₁₁	Inulobiose	0	3.98	0	0	0
104	340.3351	358.3689	25.127	C ₂₂ H ₄₄ O ₂	6-Hydroxy-8-docosanone	0.03	0.11	0.03	0.03	0.04
105	86.13	121.09	3.122	C ₅ H ₁₀ O	(S)-2-Methylbutanal	0	0	0	3.48	3.48
106	592.59	197.1204	13.065	C ₃₈ H ₇₆ N ₂ O ₂	Stearamide	0	0.26	0	0	0
107	180.16	296.1776	9.053	C ₇ H ₈ N ₄ O ₂	Paraxanthine	0	0.03	0	0	0
108	152.177	182.0707	4.364	C ₅ H ₄ N ₄ S	6-Mercaptopurine	0.02	0	0	0	0
109	453.6	270.1616	3.321	C ₂₅ H ₄₃ NO ₆	10-Deoxymethymycin	0	0.02	0.08	0.08	0.08
110	212.37	170.0134	3.122	C ₁₄ H ₂₈ O	2-Tetradecanone	0	0.58	0.05	0.04	0