Supplementary Material

Non-Targeted Metabolomics Combined with Chemometrics by UHPLC–Orbitrap–HRMS and Antioxidant Activity of *Atractylodes chinensis* (DC.) Koidez. from Eight Origins

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Table S1. Mass spectrometry identification results of chemical constituents of *Atractylodes chinensis* (DC.) Koidez.

No.	Name	Formula	Ionmode	RT [min]	Error [ppm]	MS fragment [*m/z*]	Calculate. MW	MS^2 fragments [m/z]	Classification
1	L-Tyrosine	$C_9H_{11}NO_3$	+	2.041	-2.27	182.08104	181.0735	165.05469, 147.04419, 136.07579, 123.04431, 119.04945, 91.05481	Amino acids
2	Adenosine	$C_{10}H_{13}N_5O_4$	+	2.094	-3.37	268.10333	267.0959	136.06184, 119.03561, 85.0291, 57.0342	Alkaloids
3	2'-Deoxyadenosine	$C_{10}H_{13}N_5O_3$	+	2.165	-2.91	252.1084	251.1011	136.06184, 119.03565, 117.05501, 99.04454, 73.02895	Alkaloids
4	Guanosine	$C_{10}H_{13}N_5O_5$	+	2.193	-3.25	284.09796	283.0908	153.04205, 152.05663, 135.03020, 110.0351, 109.0513	Alkaloids
5	Guanine	$C_5H_5N_5O$	+	2.194	-2.36	152.05635	151.0491	135.03018, 110.03527, 109.05110, 69.0342	Alkaloids
6	2-Furoic acid	$C_5H_4O_3$	+	2.525	-3.07	113.02352	112.0163	97.02898, 95.01339, 85.02930, 73.02917, 69.03438, 67.01877, 57.03429	Organic acids
7	L-Isoleucine	$C_6H_{13}NO_2$	+	2.565	-2.21	132.10175	131.0943	86.09708, 84.08158, 69.07080	Amino acids
8	Chlorogenic acid*	$C_{16}H_{18}O_9$	-	3.162	0.04	353.08789	354.0951	191.05499, 179.03365, 173.04413, 135.04353, 109.02770, 93.03292, 87.00679, 59.01215	Phenylpropanoids
			+	7.681	-2.84	355.10138	354.09408	163.03859, 117.03361, 145.02820	
9	Vanillic acid	$C_8H_8O_4$	+	3.912	-1.64	169.04924	168.042	155.03383, 141.05455, 139.03888, 127.03941, 111.04434, 93.03393, 81.03397, 65.03938	Phenols
10	L-Phenylalanine	$C_9H_{11}NO_2$	+	4.07	-2.3	166.08592	165.0786	131.04950, 120.08102, 103.05472, 93.07050, 91.05493, 79.0549	Amino acids
11	3-p-Coumaroylquinic acid	$C_{16}H_{18}O_8$	-	4.474	1.46	337.09341	338.1007	191.05496, 163.03871, 119.04863, 93.03274	Phenylpropanoids
			+	9.597	-1.87	339.10681	338.09955	215.06976, 148.04713, 147.04376, 119.04919,	
12	Cryptochlorogenic acid	$C_{16}H_{18}O_9$	-	5.131	0.05	353.0878	354.0951	191.05505, 179.03375, 173.04424, 135.04352, 93.03278, 85.02778	Phenylpropanoids
			+	8.198	-2.07	355.10162	354.09408	181.04922, 163.03868, 119.04919, 117.03361	
13	Neochlorogenic acid*	$C_{16}H_{18}O_9$	+	5.846	-2.84	355.10159	354.0941	193.04901, 163.03893, 145.02802, 135.04422, 117.03379, 107.04957	Phenylpropanoids
			-	3.029	0.49	353.0881	354.09525	191.05522, 179.03384, 135.04356, 134.03581	
14	5-O-Feruloylquinic acid	$C_{17}H_{20}O_9$	-	6.015	0.33	367.10342	368.1109	193.04924, 191.05504, 173.04359, 155.03311, 134.03568, 93.03281, 87.00692	Phenylpropanoids

No.	Name	Formula	Ionmode	RT [min]	Error [ppm]	MS fragment [*m/z*]	Calculate. MW	MS^2 fragments [m/z]	Classification
15	Indole-3-acrylic acid	$C_{11}H_9NO_2$	+	6.293	-2.11	188.07022	187.0629	170.0604, 146.06007, 144.08092, 143.07344, 118.06543, 117.07003, 115.05456, 91.05455	Miscellaneous
16	D-Tryptophan	$C_{11}H_{12}N_2O_2$	+	6.294	-2.51	205.09665	204.0894	188.07066, 146.06004, 144.08080, 118.06543, 132.08089, 130.06517, 115.05450, 91.05484	Amino acids
			-	5.032	1.24	203.08176	204.08894	159.09151, 142.06470, 117.05414, 116.04893,	
17	4-p-Coumaroylquinic acid	$C_{16}H_{18}O_8$	-	6.443	1.29	337.09329	338.1006	173.04424, 163.03841, 119.04894, 93.03278, 67.01717	Phenylpropanoids
			+	10.153	-1.78	339.10684	338.09954	215.06981, 197.05927, 169.06445, 147.04376	
18	Phellavin	$C_{26}H_{32}O_{12}$	-	7.473	0.5	535.18213	536.1896	373.12866, 109.02774, 89.02255, 71.01205	Flavonoids
19	4-O-Feruloylquinic acid	$C_{17}H_{20}O_9$	-	7.613	0.29	367.10336	368.1108	193.04948, 173.04424, 134.03571, 117.03310, 93.03280,67.01711, 59.01212	Phenylpropanoids
			+	10.812	-2.14	369.11722	368.11005	177.05415, 149.05942, 145.02815, 117.03344	
20	Caffeic acid	$C_9H_8O_4$	+	7.882	-2.33	181.04918	180.0418	179.03421, 163.03888, 137.05957, 135.04413, 117.03366, 107.04984, 91.05464, 89.03927	Phenols
21	3-O-Feruloylquinic acid	$C_{17}H_{20}O_9$	+	8.31	-1.69	369.11688	368.1101	177.05447, 149.05972, 145.02835, 133.02855, 117.03381	Phenylpropanoids
			-	5.672	0.28	367.10349	368.11083	193.04955, 191.03397, 175.03868, 173.04427, 149.05928	
22	Icariside F2	$C_{18}H_{26}O_{10}$	-	9.624	0.48	401.14536	402.1528	113.02279, 99.00706, 83.01206, 73.02779, 71.01208, 59.01209	Phenols
23	ar-Turmerone	$C_{15}H_{20}O$	+	10.328	-2.9	217.15807	216.1508	189.16357, 175.14807,145.10118, 133.10124, 119.08582, 105.07043, 95.08601, 81.07056	Terpenoids
24	4,6,2',4'-Tetramethoxychalcone 2'-beta-glucoside	$C_{25}H_{30}O_{11}$	-	10.985	1	505.17175	506.1793	487.16052, 475.15967, 343.11899, 89.02265, 59.01197	Flavonoids
25	D-Camphor	$C_{10}H_{16}O$	+	11.452	-2.27	153.127	152.1198	135.11683, 125.05998, 109.10164, 107.08600, 93.03409, 81.07062, 67.05423, 65.03938	Terpenoids
26	Syringaldehyde	$C_9H_{10}O_4$	+	11.628	-2.33	183.06477	182.0575	155.07031, 140.04678, 125.02361, 123.04424, 95.04968, 81.03426, 65.03938, 55.01874	Phenols

No.	Name	Formula	Ionmode	RT [min]	Error [ppm]	MS fragment [*m/z*]	Calculate. MW	MS^2 fragments [m/z]	Classification
27	4-Formylphenyl beta-D-ribopyranoside	$C_{12}H_{14}O_6$	+	11.866	-3.36	255.08545	254.0782	227.09103, 195.06525, 177.05466, 167.07024, 123.04405, 107.0493, 79.05488, 71.04996	Glycosides
28	Icariside D1	$C_{19}H_{28}O_{10}$	-	11.966	0.81	415.16135	416.1686	191.05492, 113.02245, 99.00703, 89.02268, 72.99126	Glycosides
29	Scopoletin	$C_{10}H_8O_4$	+	12.102	-2.58	193.04893	192.0418	178.02605, 165.05510, 150.03107, 149.05988, 137.05975, 133.02850, 122.03655	Phenylpropanoids
30	Abscisic acid	$C_{15}H_{20}O_4$	-	12.227	-0.3	263.12285	264.1361	245.11740, 219.13812, 203.10664, 201.12767, 163.11142, 161.09605, 135.07957	Terpenoids
31	Ferulic acid	$C_{10}H_{10}O_4$	+	12.343	-2.2	195.06487	194.0575	193.04985, 177.05466, 149.05969, 145.02847, 117.03382, 91.05466, 89.03918	Phenylpropanoids
32	Dehydrodiisoeugenol	$C_{20}H_{22}O_4$	+	12.39	-2.67	327.15826	326.1509	295.13275, 175.07626, 163.07530, 137.05972, 133.06473, 131.04929, 122.03649, 105.07018	Lignans
33	(5S,6S)-5-hydroxy-4-methoxy-6-(2-phenylethyl)-5,6-dihydro-2H-pyran-2-one	$C_{14}H_{16}O_4$	+	12.422	-3.3	249.11139	248.104	204.7819, 187.07530, 159.08058, 131.08563, 129.07022,105.07033, 93.07023, 91.05471	Lactones
34	Isofraxidin	$C_{11}H_{10}O_5$	+	12.907	-3.19	223.05937	222.0521	190.02608, 179.03410, 163.03908, 162.03108, 135.04410, 134.03612, 107.04955, 91.05439	Phenylpropanoids
35	Isochlorogenic acid B*	$C_{25}H_{24}O_{12}$	+	14.549	-1.65	517.133	516.1259	499.12405, 337.09216, 319.08051, 163.03889, 135.04414, 117.03378, 107.04945	Phenylpropanoids
			-	11.561	0.31	515.11945	516.12694	353.08810, 191.03384, 179.03369, 173.08041, 135.04355	
36	Isochlorogenic acid A*	$C_{25}H_{24}O_{12}$	+	14.8	-1.35	517.13336	516.1261	449.12115, 337.09009, 319.08017, 163.03889, 135.04411, 117.03378, 89.03913	Phenylpropanoids
			-	10.349	0.46	515.1193	516.12702	353.08786, 191.03386, 179.03375, 173.04428, 135.04352	
37	Isochlorogenic acid C	$C_{25}H_{24}O_{12}$	+	15.942	-1.23	517.1333	516.1261	500.12924, 449.12418, 163.03893, 135.04416, 117.03381, 107.04971	Phenylpropanoids
			-	9.187	0.28	515.11957	516.12692	353.08807, 335.07858, 173.08076	
38	Wikstromol	$C_{20}H_{22}O_7$	+	16.088	-2.42	375.14282	374.1357	357.13229, 345.13348, 325.10831, 161.05962, 137.05969, 107.04948, 91.05465, 73.02914	Lignans
39	2-[(2S)-6-Hydroxy-6-methyl-2-heptanyl]-5-methylphenyl alpha-D-glucopyranoside	$C_{21}H_{34}O_7$	+	16.677	-3.16	399.23642	398.2292	219.17441, 163.11218, 135.08078, 111.08079, 109.10167, 85.02901, 69.03426	Glycosides

No.	Name	Formula	Ionmode	RT [min]	Error [ppm]	MS fragment [*m/z*]	Calculate. MW	MS^2 fragments [m/z]	Classification
40	Pinoresinol 4-O-glucoside	$C_{26}H_{32}O_{11}$	-	16.858	0.17	519.18707	520.1946	357.13440, 342.11038, 122.03571, 121.02775, 83.01205, 71.01198, 59.01201	Lignans
41	Curcolonol	$C_{15}H_{20}O_4$	+	17.116	-3.33	265.14249	264.1353	229.12241, 211.11171, 201.12691, 161.05969, 149.05952, 107.04958, 81.07051	Terpenoids
42	(1S,2S)-1-(4-Hydroxy-3-methoxyphenyl)-2-{4-[(1E)-3-hydroxy-1-propen-1-yl]-2,6-dimethoxyphenoxy}-1,3-propanediol	$C_{21}H_{26}O_8$	+	17.396	-1.8	407.16931	406.162	193.08591, 150.06783, 149.05981, 133.06496, 118.04189, 107.04964, 91.05482, 79.05488	Miscellaneous
43	7-methoxy-2-methyl-2-(4-methylpent-3-enyl)-2H-chromene	$C_{17}H_{22}O_2$	+	17.442	-2.61	259.16852	258.1613	203.10684, 189.09143, 161.05980, 137.05981, 111.08081, 109.10146, 81.07052, 79.05479	Miscellaneous
44	Reynosin	$C_{15}H_{20}O_3$	+	17.571	-4.56	249.14758	248.1401	213.12767, 185.13254, 157.10129, 133.10159, 67.05490	Terpenoids
45	6-Prenylcatechin	$C_{20}H_{22}O_6$	-	17.604	0.4	357.13431	358.1418	339.12311, 150.03050, 108.01985	Flavonoids
46	7-(3,4-dihydroxyphenyl)-5-hydroxy-1-(4-hydroxyphenyl)heptan-3-one	$C_{19}H_{22}O_5$	+	17.614	-3.25	331.15292	330.1457	313.14316, 287.12796, 255.10132, 151.07541, 137.05971, 122.03635, 91.05486	Phenols
47	Carpinontriol B	$C_{19}H_{20}O_6$	+	18.771	-2.53	345.13248	344.1251	299.09189, 269.07941, 239.10619, 223.07516, 198.06816, 137.05914	Phenols
48	(1S,2R)-2-methyl-1,2,3,4-tetrahydronaphthalen-1-ol	$C_{11}H_{14}O$	+	19.478	-3.05	163.11125	162.104	145.10133, 131.04921, 117.07024, 105.07030, 103.05463, 93.07030, 91.05466, 79.05488	Miscellaneous
49	Methyl ferulate	$C_{11}H_{12}O_4$	+	19.854	-3.29	209.08017	208.0729	177.05435, 149.05963, 125.05978, 121,06503, 106.04172, 91.05474, 78.04709, 65.03938	Phenylpropanoids
50	Selina-4(14),7(11)-dien-8-one	$C_{15}H_{22}O$	+	20.744	-3.7	219.17343	218.1663	201.16389, 163.11189, 161.13264, 149.09613, 123.11708, 111.08082, 107.08575, 95.08624	Terpenoids
51	2-[(2'E)-3',7'-dimethyl-2',6'-octadienyl]-4-methoxy-6-methylphenol	$C_{18}H_{26}O_2$	+	21.289	-3.27	275.19962	274.1924	257.18979, 229.19518, 133.10126, 119.08578, 107.08574, 105.07025, 91.05483	Polyacetylene

No.	Name	Formula	Ionmode	RT [min]	Error [ppm]	MS fragment [*m/z*]	Calculate. MW	MS^2 fragments [m/z]	Classification
52	4-hydroxy-6-[2-(2-methyl-1,2,4a,5,6,7,8,8a-octahydronaphthalen-1-yl)ethyl]oxan-2-one	$C_{18}H_{28}O_3$	+	21.293	-3.11	293.21011	292.2029	275.20056, 257.18918, 147.11691, 109.06512, 107.08605, 81.07047, 79.05496	Lactones
53	Caryophyllene oxide	$C_{15}H_{24}O$	+	21.493	-3.59	221.18929	220.1819	203.17961, 175.14815, 163.14832, 161.13274, 147.11690, 109.10161, 95.08611, 81.07054	Terpenoids
54	7-Demethylsuberosin	$C_{14}H_{14}O_3$	+	22.087	-3.2	231.10097	230.0936	175.03903, 163.03931, 131.04935, 119.04976, 91.05491, 69.07069, 53.00300	Coumarins
55	Pinosylvin	C14H12O2	+	22.103	-2.81	213.09036	212.0831	167.08551, 109.02872, 103.05459, 91.0545, 81.03417	Phenols
56	Limonin	$C_{26}H_{30}O_8$	+	22.179	-1.59	471.20053	470.1933	453.19058, 139.03896, 111.04443, 93.03391	Terpenoids
57	Sedanolide	$C_{12}H_{18}O_2$	+	22.38	-2.56	195.13745	194.1302	177.12744, 149.13307, 135.04459, 107.08617, 93.07049, 81.07054, 67.05494	Phthalides
58	octadecatetraenoic acid	$C_{18}H_{28}O_2$	+	22.383	-3.48	277.21512	276.208	259.20566, 163.11162, 161.13290, 133.10107, 119.08583, 93.07054, 81.07060, 79.05486	Organic acids
59	Arctigenin	$C_{21}H_{24}O_6$	+	22.658	-2.59	373.16339	372.1563	355.15503, 313.14279, 189.09081, 151.07533, 137.05975, 122.03642, 91.05475	Lignans
60	(4E,6E,12E)-tetradecatriene-8,10-diyne-1,3-diol-diacetate	$C_{18}H_{20}O_4$	+	23.341	-2.47	301.14285	300.1354	183.08073, 153.06950, 128.06212, 115.05444, 91.05468, 83.04979, 65.03925, 55.05502	Polyacetylene
61	(9Z,11E,15Z)-13-hydroxy-9,11,15-octadecatrienoic acid	$C_{18}H_{30}O_3$	+	23.516	-3.57	295.22571	294.2184	259.20779, 165.12743, 121.10123, 111.08066, 81.07054, 79.05496, 67.05501	Organic acids
62	Tetraneurin A	$C_{17}H_{22}O_6$	+	23.77	-2.88	323.14819	322.1407	203.10699, 155.07065, 95.04971, 79.05489, 69.03425, 67.05506, 55.01873	Terpenoids
63	Saussureamine B	$C_{20}H_{27}NO_4$	+	24.167	-2.84	346.20035	345.193	231.13791, 213.12729, 163.07541, 116.07098, 79.05499, 70.06595, 69.07061	Terpenoids
64	(6E,12E)-Tetradecadiene-8,10-diyne-1,3-diol	$C_{14}H_{18}O_2$	+	24.232	-3.35	219.13716	218.13	201.12755, 147.08022, 131.08591, 117.07021, 91.05482, 69.03435, 67.05505	Polyacetylene
65	7-phenyl-2-heptene-4,6-diyn-1-ol	$C_{13}H_{10}O$	+	24.63	-2.57	183.07991	182.0727	165.06970, 153.07001, 141.06985, 127.05453, 103.05456, 77.03942	Polyacetylene
66	Atractyloyne	$C_{19}H_{24}O_4$	+	24.774	-2.24	317.1741	316.1668	199.11232, 157.06467, 10106036, 91.05487, 83.04984, 67.05494, 55.05516	Polyacetylene

No.	Name	Formula	Ionmode	RT [min]	Error [ppm]	MS fragment [*m/z*]	Calculate. MW	MS^2 fragments [m/z]	Classification
67	1,7-bis(4-hydroxyphenyl)heptan-3-one	$C_{19}H_{22}O_3$	+	24.779	-2.9	299.16327	298.156	157.06470, 145.06479, 121.06526, 115.05467, 103.05462, 91.05483, 83.04986, 79.05495	Phenols
68	5-Hydroxymethylfurfural	$C_6H_6O_3$	+	24.809	-0.86	127.03877	126.0316	109.02885, 99.04475, 85.02895, 81.03416, 71.04996, 67.01865, 53.00322	Miscellaneous
69	Atractylenolide III*	$C_{15}H_{20}O_3$	+	25.01	-4.02	249.14754	248.1403	231.13794, 189.09100, 185.13263, 163.07533, 149.06004, 105.07038, 93.07052, 69.07064	Terpenoids
			-	25.001	-1.73	247.13351	248.14082	203.14348, 187.11194, 147.07993	
70	Furanodienone	$C_{15}H_{18}O_2$	+	25.014	-4.06	231.13687	230.1297	213.12697, 175.07526, 163.07527, 161.05975, 119.08567, 95.08593, 93.07043, 69.07084	Terpenoids
			-	24.889	-2.14	229.12303	230.13019	179.03377, 122, 94,91	
71	4-Methoxycinnamaldehyde	$C_{10}H_{10}O_2$	+	25.015	-2.14	163.07465	162.0677	161.05959, 135.08040, 131.04906, 115.05490, 107.04958, 105.07030, 91.05482, 79.05498	Phenylpropanoids
72	2-(biphenyl-4-yl)acetaldehyde	$C_{14}H_{12}O$	+	25.036	-2.98	197.09546	196.0882	178.07758, 152.06200,103.05472, 91.05478, 65.03915	Miscellaneous
73	8-Epiiridodial glucoside	$C_{16}H_{26}O_7$	+	26.238	-3.41	331.17407	330.1667	127.03918, 97.02892, 85.06548, 69.03432, 57.07081	Terpenoids
74	Atractylenolide II*	$C_{15}H_{20}O_2$	+	26.345	-3.78	233.15263	232.1455	215.14339, 189.14825, 177.09103, 151.07529, 133.06502, 105.07033, 95.08626, 81.07050	Terpenoids
75	Acetylatractylodinol	$C_{15}H_{12}O_3$	+	26.39	-3.27	241.08517	240.0779	213.09074, 199.07545, 198.06767, 169.06483, 171.08006, 147.04347, 93.03371, 81.03414	Miscellaneous
76	Atractylenolide I*	$C_{15}H_{18}O_2$	+	27.147	-2.71	231.13731	230.1301	213.12764, 185.13251, 157.10117, 143.08565, 142.07767, 131.08542, 129.07039, 95.08589	Terpenoids

*Identified by standard substances.

Table S2. List of the characteristic compounds to discriminate AC according to the geographical origin

Model	Marker name	VIP score	p(corr) value	Log_2(FC)
M2	Chlorogenic acid	4.13	-0.87	2.15
	Isochlorogenic acid A	1.40	-0.93	2.14
	4,6,2',4'-Tetramethoxychalcone 2'-beta-glucoside	1.35	-0.92	1.95
	Isochlorogenic acid B	1.27	-0.92	1.85
M3	Scopoletin	5.87	-0.97	3.47
	Atractylenolide II	1.88	-0.81	1.79
M4	L-Phenylalanine	4.38	-0.96	2.40
	L-Isoleucine	2.75	-0.99	3.13
	Guanine	1.25	0.84	-7.48
	L-Tyrosine	1.05	-0.93	2.90
M5	Adenosine	3.10	-0.90	1.97

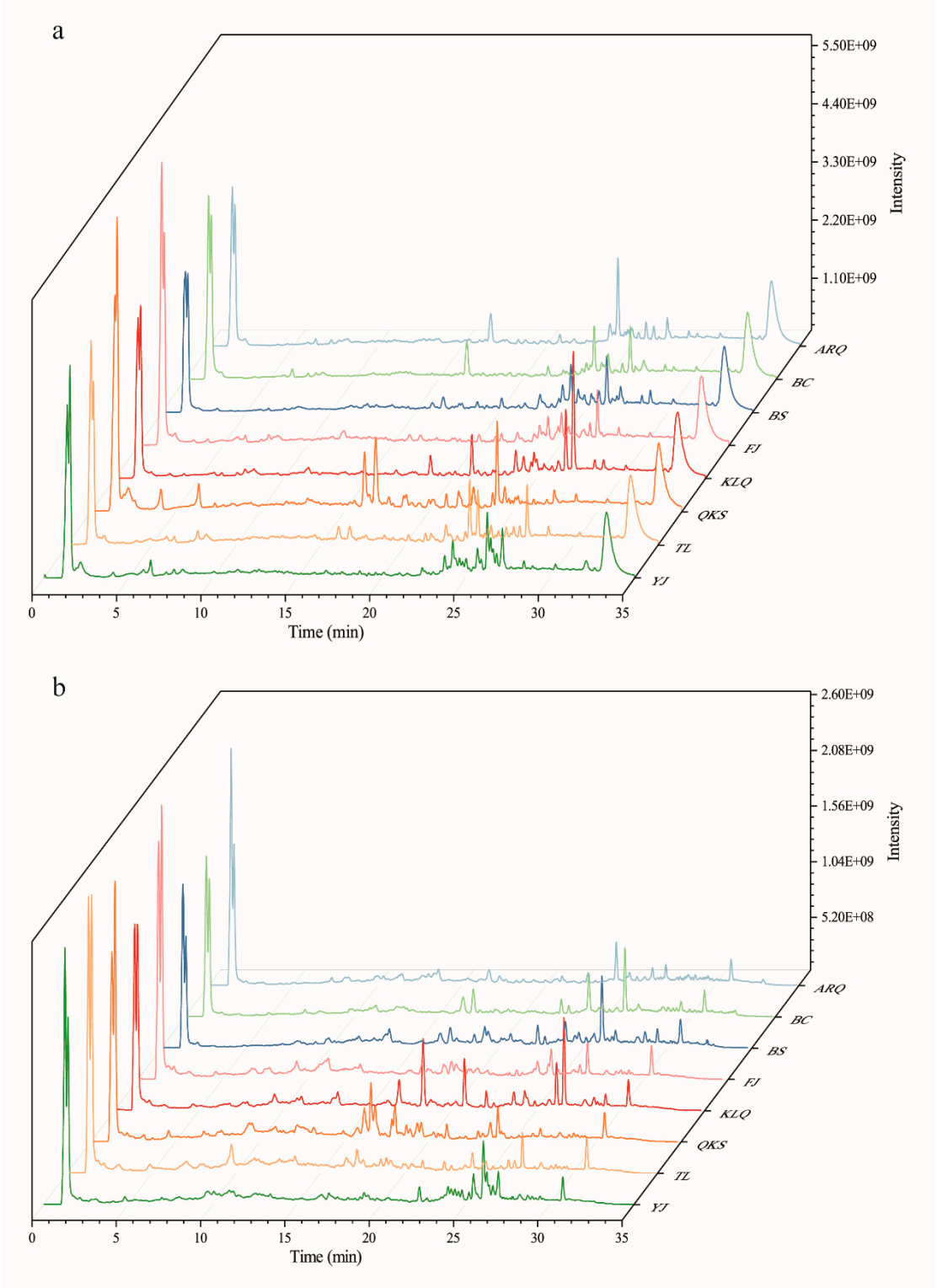
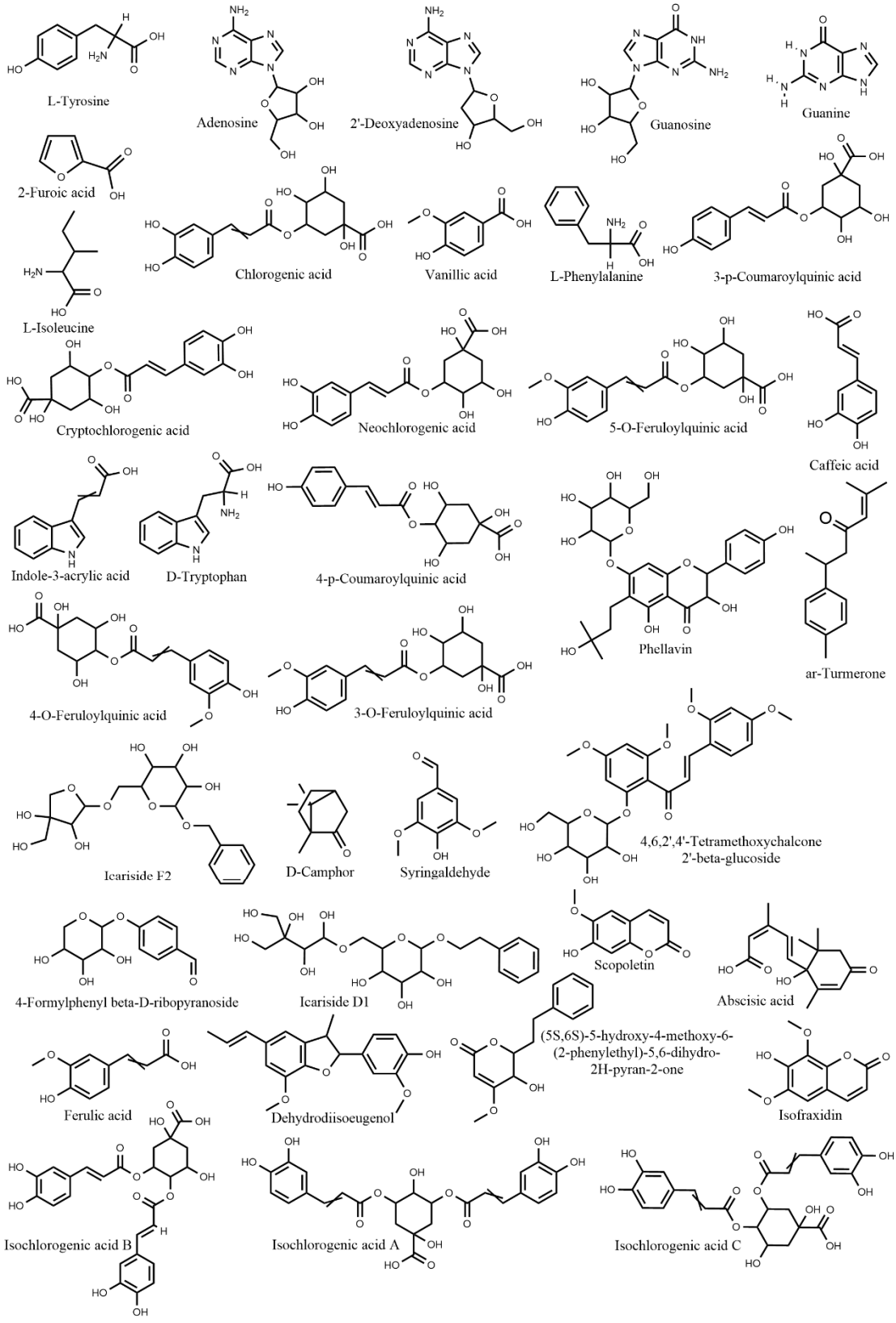


Figure S1. The total ion chromatograms of the UHPLC-Orbitrap-HRMS analysis of *Atractylodes chinensis* (DC.) Koidez. samples, with a focus on the (a) negative ion and (b) positive ion.


L-Tyrosine
Adenosine
2'-Deoxyadenosine
Guanosine
Guanine
2-Furoic acid
Chlorogenic acid
Vanillic acid
L-Phenylalanine
3-p-Coumaroylquinic acid
L-Isoleucine
Cryptochlorogenic acid
Neochlorogenic acid
5-O-Feruloylquinic acid
Caffeic acid
Indole-3-acrylic acid
D-Tryptophan
4-p-Coumaroylquinic acid
Phellavin
ar-Turmerone
4-O-Feruloylquinic acid
3-O-Feruloylquinic acid
Icariside F2
D-Camphor
Syringaldehyde
4,6,2',4'-Tetramethoxychalcone 2'-beta-glucoside
4-Formylphenyl beta-D-ribopyranoside
Icariside D1
Scopoletin
Abscisic acid
(5S,6S)-5-hydroxy-4-methoxy-6-(2-phenylethyl)-5,6-dihydro-2H-pyran-2-one
Ferulic acid
Dehydrodiisoeugenol
Isofraxidin
Isochlorogenic acid B
Isochlorogenic acid A
Isochlorogenic acid C

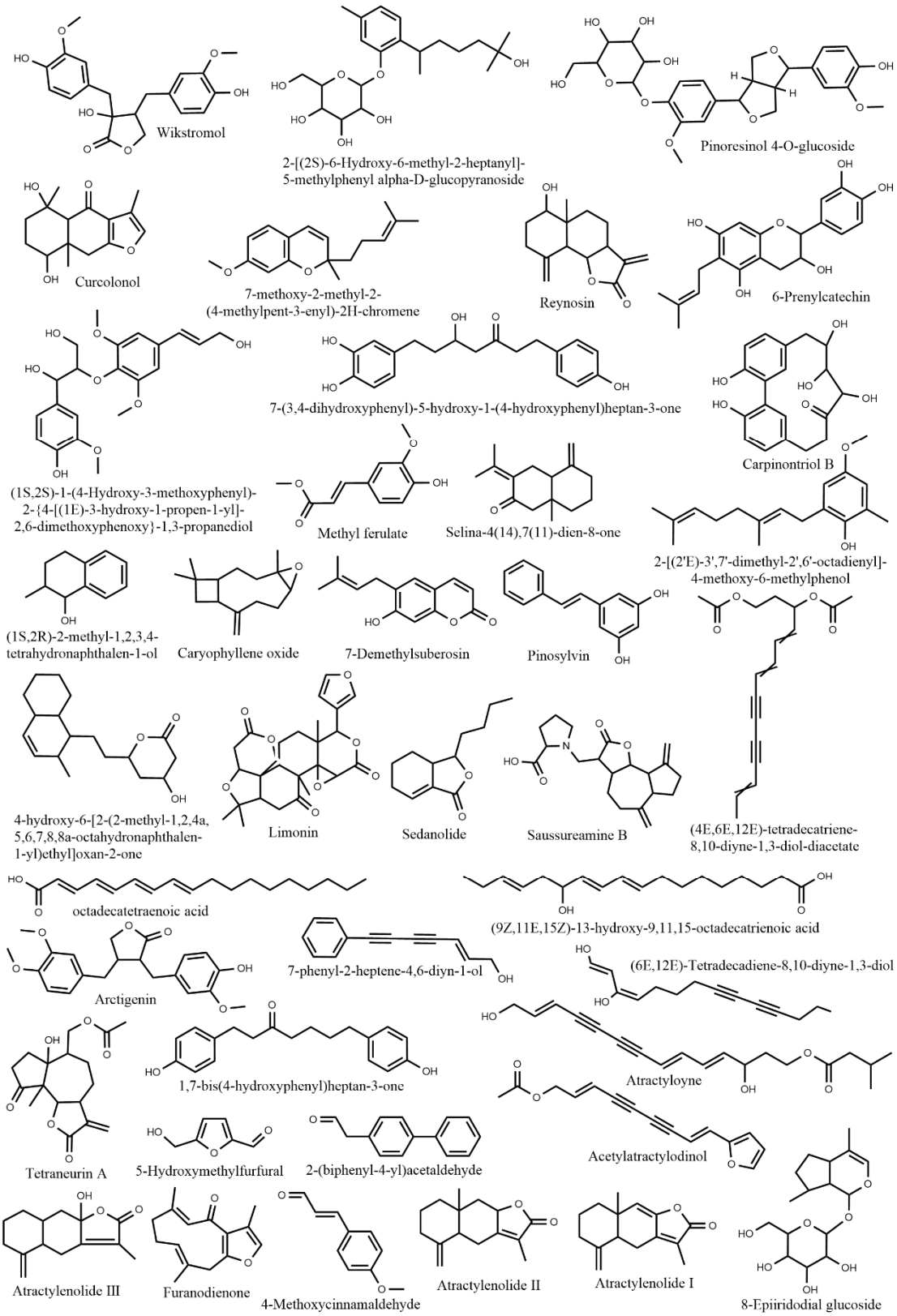


Figure S2. The chemical structure of 76 compounds identified in this study.

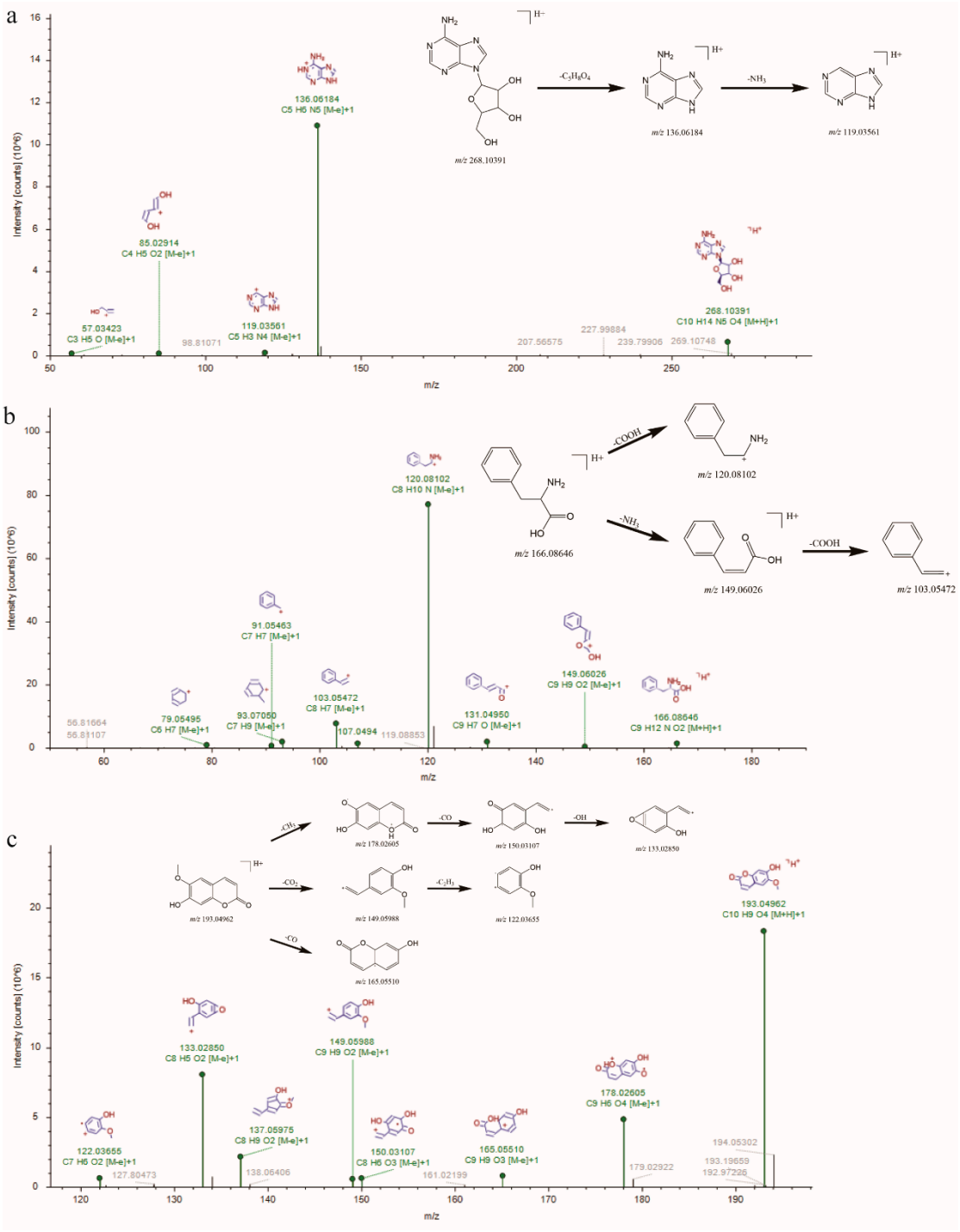


Figure S3. Mass spectrometric fragmentation patterns of (a) Adenosine, (b) L-Phenylalanine, and (c) Scopoletin.

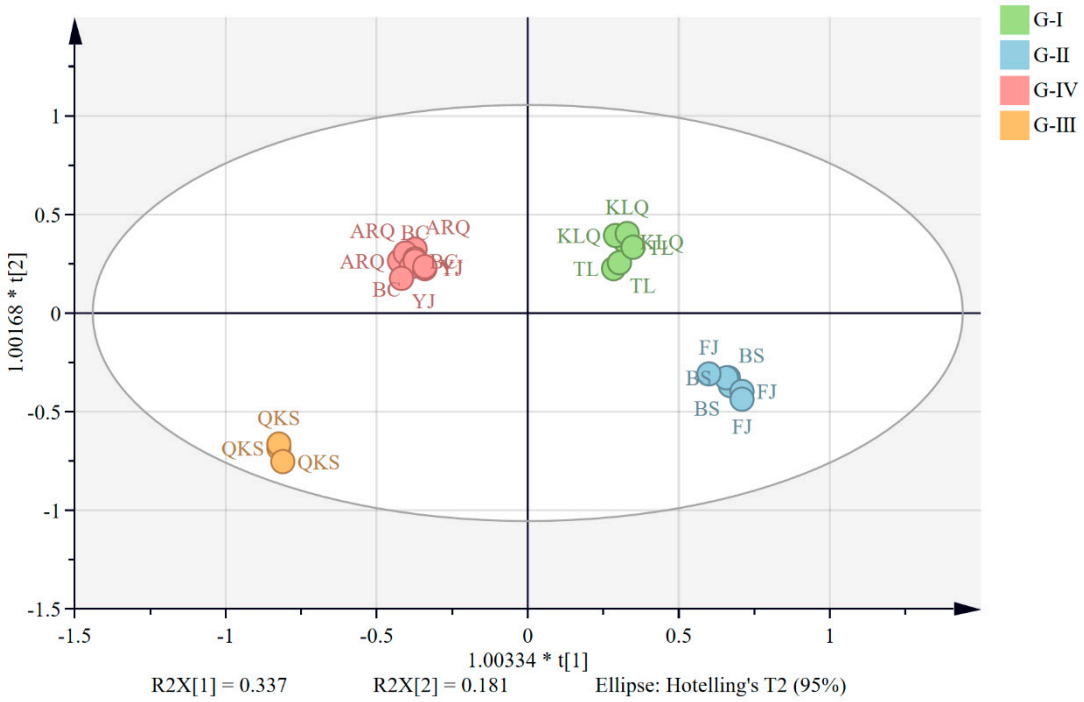


Figure S4. OPLS-DA results of AC from 8 different regions with grouping.