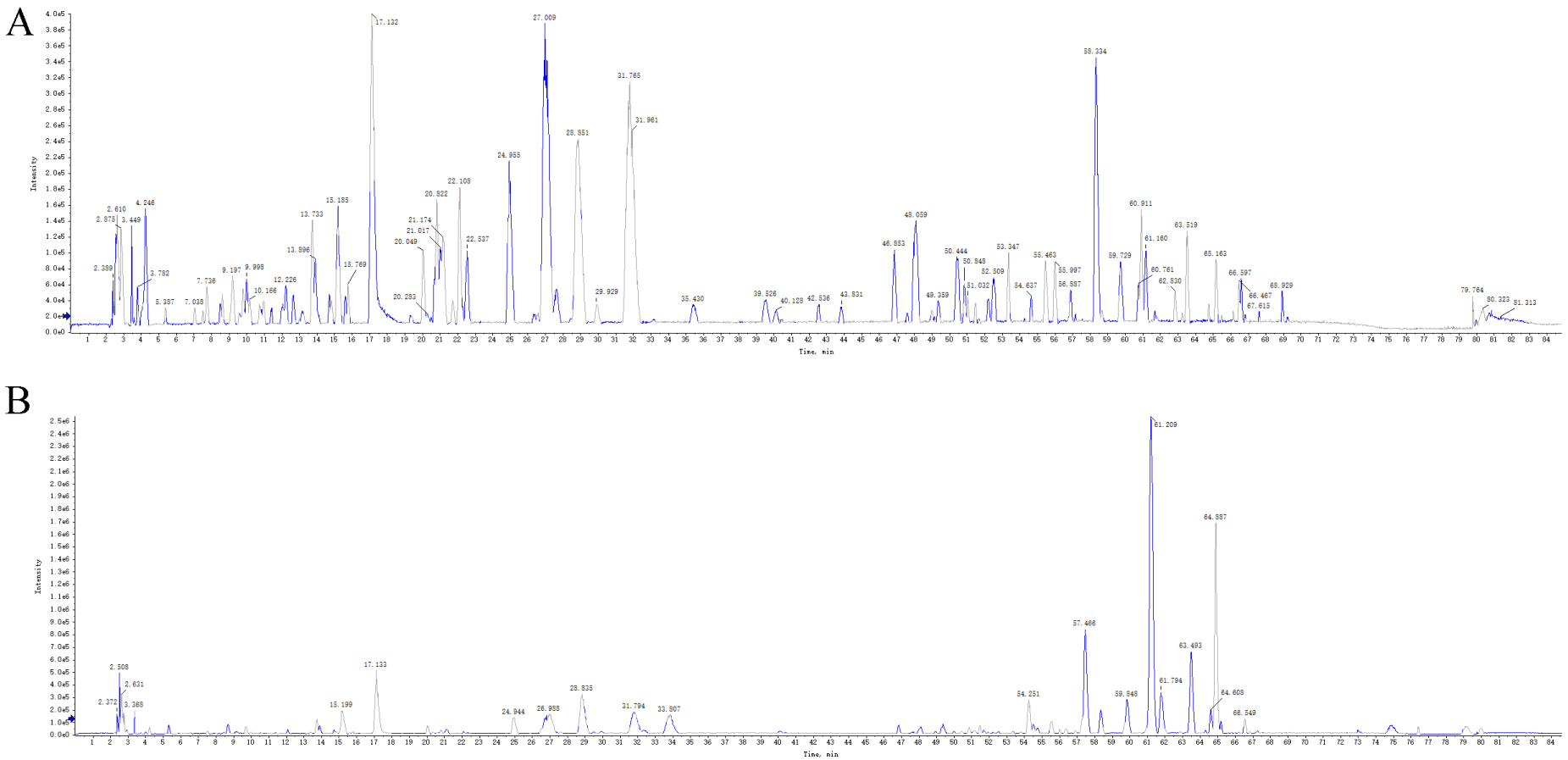

Figure S1. UPLC-MS/MS analyzed BSS-derived 10ACs. Total ion chromatogram of (A) negative and (B) positive ion model. Fingerprint of 121 components peak time,peak area and peak height etc in Supplement Table S1 and S2.

Table S1. BSS-derived 98 phytochemicals in negative mode.

Number	Index	Time (min)	Area	% Area	Height	Start (min)	End (min)	Width (min)	Width at 50% (min)	molecular ion peak
1	13	2.388589426	245394.3184	0.309800564	59595.28036	2.3406	2.4834	0.1428	0.081907565	96.9623
2	14	2.609839947	1554108.776	1.962000499	141094.8864	2.4834	2.769766667	0.286366667	0.199917997	191.0571
3	15	2.874690164	1059065.843	1.337028492	123676.0489	2.769766667	3.126366667	0.3566	0.136807687	191.021
4	17	3.449069216	412533.5864	0.52080724	125560.673	3.367716667	3.53785	0.170133333	0.051579767	191.0211
5	19	3.781898132	282304.879	0.356398678	48333.91541	3.684816667	3.927566667	0.24275	0.085911031	191.0211
6	20	4.245619288	1512411.193	1.909358959	147124.5226	3.927566667	4.43115	0.503583333	0.13944936	169.0155
7	23	5.387058259	118987.2325	0.150216647	21308.05019	5.264916667	5.483066667	0.21815	0.087876001	315.0734
8	30	7.03835752	126573.659	0.159794209	21033.26506	6.919866667	7.141266667	0.2214	0.103601505	353.0885
9	32	7.510125126	77517.94399	0.09786332	16449.63747	7.406633333	7.5765	0.169866667	0.076080715	358.0776
10	33	7.73634527	357195.944	0.450945668	46250.65933	7.5765	7.886966667	0.310466667	0.12078568	313.0572
11	37	8.498952122	152768.2606	0.192863851	26091.37989	8.368716667	8.561733333	0.193016667	0.102121768	443.1316
12	38	8.621480095	221188.9399	0.279242237	38500.18466	8.561733333	8.825783333	0.26405	0.095382374	543.1171
13	41	9.197262554	620367.443	0.783189215	60371.39525	8.946616667	9.4065	0.459883333	0.1699959	385.0777
14	42	9.621585183	145519.114	0.183712092	14125.18409	9.4065	9.717133333	0.310633333	0.187043138	558.1466
15	43	9.805449018	351440.2251	0.443679302	45827.41191	9.717133333	9.907966667	0.190833333	0.137797209	165.0571
16	44	9.997709818	450774.3205	0.569084645	57813.14242	9.907966667	10.09876667	0.1908	0.139658553	353.0881
17	45	10.1658928	254824.43	0.321705705	32297.964	10.09876667	10.31215	0.213383333	0.142919242	385.078
18	48	10.76301506	235594.0992	0.297428177	24911.20681	10.64858333	10.88716667	0.238583333	0.188763056	385.0777
19	49	10.96244543	216747.7063	0.273635356	30052.51017	10.88716667	11.12405	0.236883333	0.127219762	353.0886
20	50	11.40572845	117744.4	0.148647621	19729.52178	11.29235	11.48361667	0.191266667	0.102286581	609.1457
21	51	12.04557603	240936.3141	0.304172511	25866.87899	11.86845	12.13781667	0.269366667	0.189174479	548.1265
22	52	12.22561883	422621.9059	0.533543342	48880.41616	12.13781667	12.39925	0.261433333	0.142366758	385.0774
23	53	12.64878717	309732.7705	0.3910253	35814.32432	12.5193	12.83041667	0.311116667	0.140595795	179.0366
24	56	13.18743491	184492.8555	0.23291489	16901.91738	13.04716667	13.34395	0.296783333	0.195349031	313.0574

25	57	13.73291472	1010803.54	1.276099254	130269.1645	13.56103333	13.82316667	0.262133333	0.138067787	593.1517
26	58	13.89604192	746884.4522	0.942911906	81853.78967	13.82316667	14.22698333	0.403816667	0.151174984	421.1642
27	61	14.70048807	198611.0802	0.250738587	36515.06937	14.61355	14.75746667	0.143916667	0.103135034	623.1627
28	62	14.82009961	212443.9733	0.268202064	28784.48428	14.75746667	14.948	0.190533333	0.134992228	677.1867
29	64	15.1854123	1640830.98	2.071483831	148317.7013	14.99575	15.44565	0.4499	0.174718161	525.1617
30	65	15.61507118	233274.2191	0.294499421	34888.94395	15.49323333	15.6856	0.192366667	0.118476958	499.1952
31	66	15.76887788	328621.9374	0.414872122	49728.94215	15.6856	15.9006	0.215	0.108238568	779.2035
32	73	17.1320616	6434432.711	8.123215302	388313.0411	16.89078333	17.98188333	1.0911	0.244692991	525.1613
33	74	18.08551937	162288.0515	0.204882208	11212.77284	17.98188333	18.34153333	0.35965	0.319664609	515.1319
34	78	19.35182304	102950.1285	0.129970441	9857.228976	19.21125	19.5008	0.28955	0.194032346	807.214
35	79	20.04863894	838721.0498	1.058851957	91966.07491	19.91248333	20.22338333	0.3109	0.149207866	427.161
36	80	20.28267832	101141.2848	0.127686848	11584.37093	20.22338333	20.4385	0.215116667	0.176511343	612.1576
37	82	20.82181662	1574086.614	1.987221725	155328.4994	20.58305	20.91576667	0.332716667	0.148864393	649.2507
38	83	21.01734122	797878.0946	1.007289351	95430.40597	20.91576667	21.08145	0.165683333	0.165683333	549.1615
39	84	21.17371152	1286857.836	1.62460682	109450.5587	21.08145	21.43541667	0.353966667	0.201233258	417.1194
40	85	21.73308758	283421.0635	0.357807817	30708.88284	21.43541667	21.91426667	0.47885	0.145125782	561.1257
41	86	22.10753851	1683082.294	2.124824434	172399.2785	21.91426667	22.36516667	0.4509	0.147865202	595.1656
42	87	22.53674947	979727.7049	1.236867249	92003.37041	22.36516667	22.76783333	0.402666667	0.184275989	631.1642
43	105	24.95513973	2875661.441	3.63040816	204369.5327	24.72465	25.27035	0.5457	0.239058233	615.1477
44	107	26.40059564	134008.9836	0.16918101	11548.04563	26.23033333	26.51781667	0.287483333	0.163367724	631.1658
45	108	26.56760658	75943.342	0.095875448	12890.65444	26.51781667	26.66048333	0.142666667	0.104585076	577.1547
46	109	27.00923161	8577486.778	10.8287358	376682.8086	26.66048333	27.43983333	0.77935	0.40283701	579.1699
47	110	27.62249658	670756.6598	0.846803597	43266.72655	27.43983333	27.88875	0.448916667	0.25981142	469.0898
48	114	28.85103185	5643129.24	7.124226152	231811.4227	28.51011667	29.3839	0.873783333	0.407099554	609.1807
49	116	29.9289844	297525.745	0.375614416	23921.75408	29.71785	30.17138333	0.453533333	0.203545	651.1564
50	125	31.76466851	5171777.474	6.5291633	302899.2569	31.36795	31.88885	0.5209	0.297995434	609.1811

51	126	31.96097865	3224926.094	4.07134089	241875.3571	31.88885	32.45471667	0.565866667	0.215344584	609.1806
52	146	35.42957374	400382.8835	0.505467461	23461.79379	35.21473333	35.73773333	0.523	0.279230414	693.2735
53	169	39.52583592	488933.03	0.617258498	29782.31815	39.31298333	39.83423333	0.52125	0.281201517	711.2828
54	170	40.12767936	205125.5	0.258962783	16369.24363	39.90528333	40.33311667	0.427833333	0.225066004	445.0749
55	183	42.53636979	201786.2945	0.254747169	22706.19247	42.40906667	42.695	0.285933333	0.149189294	633.2522
56	188	43.83057024	214716.9955	0.271071664	20703.89339	43.6744	43.98315	0.30875	0.183120621	417.0808
57	214	46.85268562	954040.8496	1.204438616	93020.2684	46.54578333	47.04536667	0.499583333	0.168299644	629.1603
58	219	47.59147841	84397.8165	0.106548886	12094.15475	47.49973333	47.71426667	0.214533333	0.120854637	417.0806
59	221	48.05941542	2130115.143	2.689185621	128602.3817	47.81005	48.3545	0.54445	0.306185139	656.1804
60	228	48.99514003	128482.383	0.162203897	15711.04202	48.83295	49.09481667	0.261866667	0.13017257	417.0814
61	230	49.3592165	252448.7755	0.318706535	27251.34093	49.23761667	49.50023333	0.262616667	0.151270674	762.3577
62	238	50.44378088	1120036.36	1.414001343	82387.14022	50.14716667	50.66743333	0.520266667	0.21834426	271.061
63	239	50.84777077	405139.6911	0.511472741	49951.51467	50.71471667	50.97541667	0.2607	0.135284236	629.1843
64	240	51.03209623	173698.9634	0.219288031	31715.47718	50.97541667	51.16461667	0.1892	0.090795875	983.4436
65	243	51.46867162	174082.5155	0.21977225	25720.39178	51.35566667	51.59453333	0.238866667	0.112303935	723.2122
66	246	52.20348376	262005.113	0.330771031	29872.38724	51.9753	52.35616667	0.380866667	0.134693707	371.1496629
67	247	52.50928079	637940.7725	0.805374845	56777.80229	52.35616667	52.68846667	0.3323	0.196405952	879.3997121
68	253	53.34660968	602135.6	0.760172239	87872.18138	53.21378333	53.52216667	0.308383333	0.114839465	838.3891861
69	265	54.63673416	209304.56	0.26423868	33295.55333	54.5474	54.7374	0.19	0.108432385	738.3559
70	271	55.46294461	789956.333	0.997288442	78088.56324	55.33295	55.6649	0.33195	0.177496671	329.2327
71	273	55.9965856	665050.458	0.839599744	77068.68744	55.87881667	56.16281667	0.284	0.138002135	991.5262958
72	276	56.88700899	327556.888	0.413527539	40721.02086	56.63806667	57.04161667	0.40355	0.123366694	971.5148345
73	278	57.15481454	40295.524	0.050871496	9358.030954	57.08903333	57.2791	0.190066667	0.06586124	837.3861381
74	286	58.33404759	4031691.126	5.089849644	331833.0502	58.13565	58.58385	0.4482	0.210716218	821.3908328
75	287	58.66728332	86521.31072	0.109229713	13838.21925	58.58385	58.77305	0.1892	0.103469528	205.0875438
76	291	59.72854742	848217.023	1.070840245	75967.76988	59.5587	59.9611	0.4024	0.185287929	515.1885

77	294	60.76123765	337560.0271	0.426156104	48574.30152	60.60368333	60.81805	0.214366667	0.123508574	531.2195
78	295	60.91145951	1086062.641	1.371110874	142056.8819	60.81805	61.0537	0.23565	0.129873738	821.3911
79	296	61.16018667	828944.6769	1.046509675	90429.70568	61.0537	61.36023333	0.306533333	0.149491952	825.4584
80	298	61.68044612	73879.07923	0.093269398	13357.27242	61.54981667	61.76341667	0.2136	0.086425398	821.3924
81	304	62.8303392	313249.669	0.395465244	38910.12042	62.57185	63.0232	0.45135	0.123191391	825.4603
82	305	63.24190437	82369.3945	0.103988083	11505.35728	63.0232	63.35595	0.33275	0.096423587	867.4698
83	306	63.518548	964591.9375	1.217758945	115788.5078	63.35595	63.68681667	0.330866667	0.131869269	825.4595
84	313	64.74381349	157496.8116	0.198833459	24128.00898	64.54116667	64.94541667	0.40425	0.0784919	367.1171
85	314	65.16273654	656794.9878	0.829177541	80671.42168	64.94541667	65.30093333	0.355516667	0.127513218	867.4696
86	316	65.48160533	29465.982	0.03719963	8663.172268	65.3954	65.56151667	0.166116667	0.052218686	809.4647
87	321	66.14887748	68068.804	0.085934157	13549.24527	66.0134	66.27521667	0.261816667	0.070768277	867.4669
88	323	66.46720509	277794.9128	0.350705025	52628.09946	66.37013333	66.53625	0.166116667	0.088639754	867.4696
89	324	66.59722229	346594.1732	0.437561354	54983.02688	66.53625	66.74833333	0.212083333	0.109543904	353.1015
90	325	66.81886211	44000.0385	0.055548298	9758.133365	66.74833333	66.8908	0.142466667	0.084085259	909.4791
91	332	67.61535977	57317.08	0.072360533	13546.89778	67.55538333	67.69821667	0.142833333	0.066972403	311.2219
92	344	68.9292563	211177.8595	0.266603646	39158.66929	68.86206667	69.02746667	0.1654	0.087860028	351.0861
93	400	79.76365529	120851.145	0.152569762	40192.79341	79.71508333	79.85666667	0.141583333	0.060685462	209.9497
94	402	80.32331815	346566.4473	0.437526351	21334.68849	80.05033333	80.52881667	0.478483333	0.278549881	61.9925
95	403	80.63162173	77465.36051	0.097796936	11853.57456	80.52881667	80.67255	0.143733333	0.110621302	96.9627
96	404	80.77506781	198687.3695	0.250834899	17480.75033	80.67255	80.9595	0.28695	0.28695	96.9626
97	405	81.04446775	99577.74516	0.125712942	9108.922323	80.9595	81.17463333	0.215133333	0.215133333	96.9626
98	406	81.31303177	93860.07924	0.118494616	8036.585736	81.17463333	81.4618	0.287166667	0.203089547	96.9626

Table S2. BSS-derived 26 phytochemicals in positive mode.

Number	Index	Time (min)	Area	% Area	Height	Start (min)	End (min)	Width (min)	Width at 50% (min)	molecular ion peak
1	9	2.372159373	617027.5866	0.438804304	159630.3103	2.33635	2.455566667	0.119216667	0.065689908	175.1184
2	10	2.507827696	1515179.538	1.077532539	486908.1617	2.455566667	2.57455	0.118983333	0.046608864	381.0791
3	11	2.631491937	2582906.293	1.836855307	315281.9256	2.57455	2.862216667	0.287666667	0.185491379	144.1017
4	13	3.36836496	576937.4745	0.410293887	188135.5947	3.308733333	3.481533333	0.1728	0.05042743	268.1035
5	71	15.19855203	2353678.222	1.673837857	183293.5127	14.97716667	15.47838333	0.501216667	0.221634894	503.1511
6	81	17.13254996	6152326.769	4.375278387	502844.7263	16.84933333	17.88526667	1.035933333	0.182735661	503.1506
7	120	24.94364556	1759687.599	1.251416481	131260.3541	24.74896667	25.22858333	0.479616667	0.214876753	581.1839
8	127	26.70590498	1313008.832	0.933757159	123569.5998	26.37091667	26.75775	0.386833333	0.149307313	463.1562
9	128	26.80212609	683508.6609	0.486082873	144380.5353	26.75775	26.85266667	0.094916667	0.094916667	463.1559
10	129	26.98791406	2861284.115	2.034826013	155303.4052	26.85266667	27.46978333	0.617116667	0.299570132	581.1839
11	139	28.83514816	6076891.579	4.321632024	314692.0716	28.5301	29.29053333	0.760433333	0.306731792	611.1951
12	156	31.79406366	4248248.188	3.021177056	169670.2978	31.37758333	32.2114	0.833816667	0.415848838	611.1948
13	162	33.80680935	3736182.6	2.657017352	146529.7813	33.43041667	34.3543	0.923883333	0.391744261	261.1121
14	266	54.2507346	2836239.342	2.017015214	269682.7625	54.0621	54.41666667	0.354566667	0.174505269	373.1283
15	281	57.46562905	10484319.02	7.456010733	829979.1235	57.1221	57.78458333	0.662483333	0.180403612	373.1273
16	284	58.35080692	1995386.293	1.41903557	189632.5232	58.16655	58.6179	0.45135	0.171144309	343.1174
17	294	59.84789674	3491585.691	2.483070224	271213.621	59.55078333	60.09681667	0.546033333	0.18655747	403.1378
18	303	61.20899279	35197822.33	25.0312243	2522995.883	60.8131	61.5944	0.7813	0.219009718	403.1368
19	304	61.79430709	4261401.591	3.030531209	327649.4267	61.5944	62.2072	0.6128	0.205061076	343.1171
20	310	63.49347757	7797682.322	5.545386683	653869.6579	63.1374	63.75558333	0.618183333	0.190377917	433.148
21	314	64.60752385	1584369.642	1.126737658	191512.1808	64.42408333	64.73315	0.309066667	0.136396436	419.133
22	315	64.88742729	14743011.77	10.48461553	1678893.842	64.73315	65.11155	0.3784	0.130424993	373.1271
23	324	66.54903153	948909.0956	0.674824601	119444.5677	66.40573333	66.73921667	0.333483333	0.12431931	389.1223