

## Supporting information

Table S1. Stability (A) and Repeatability (B) of UPLC-Q-TOF/MS method

A:

NO.	Positive mode				NO.	Negative mode			
	RT (min)	RSD (%)	<i>m/z</i>	RSD (%)		RT (min)	RSD (%)	<i>m/z</i>	RSD (%)
1	0.63	0.8413	229.1522	0.0005	11	0.59	0.4237	267.0722	0.0004
2	2.52	0.2024	218.2117	0.0003	12	2.18	0.1972	201.0223	0.0002
3	2.60	0.1308	260.2384	0.0006	13	4.82	0.0726	265.1481	0.0008
4	4.36	0.0849	318.3002	0.0004	14	5.52	0.0507	524.2751	0.0002
5	5.20	0.0500	302.3044	0.0001	15	6.01	0.0749	540.3306	0.0005
6	5.53	0.0886	544.3409	0.0002	16	6.37	0.0644	485.2828	0.0003
7	5.94	0.0286	496.3391	0.0003	17	7.04	0.0526	568.3621	0.0005
8	6.93	0.0620	524.3715	0.0007	18	7.54	0.0371	327.2371	0.0006
9	7.55	0.0331	637.3090	0.0003	19	7.71	0.0220	303.2316	0.0009
10	8.79	0.8413	621.3092	0.0002	20	8.78	0.0353	423.3271	0.0003

B:

NO.	Positive mode				NO.	Negative mode			
	RT (min)	RSD (%)	<i>m/z</i>	RSD (%)		RT (min)	RSD (%)	<i>m/z</i>	RSD (%)
1	0.63	0.3651	229.1522	0.0003	11	0.59	0.7966	267.0722	0.0021
2	2.52	0.1825	218.2117	0.0003	12	2.18	0.2569	201.0223	0.0005
3	2.60	0.1500	260.2384	0.0005	13	4.82	0.0934	265.1481	0.0006
4	4.36	0.0872	318.3002	0.0003	14	5.52	0.0417	524.2751	0.0008
5	5.20	0.0653	302.3044	0.0004	15	6.01	0.0549	540.3306	0.0010
6	5.53	0.0759	544.3409	0.0008	16	6.37	0.0738	485.2828	0.0010
7	5.94	0.0471	496.3391	0.0010	17	7.04	0.0497	568.3621	0.0005
8	6.93	0.0880	524.3715	0.0007	18	7.54	0.0531	327.2371	0.0010
9	7.55	0.0265	637.3090	0.0006	19	7.71	0.0298	303.2316	0.0004
10	8.79	0.0432	621.3092	0.0013	20	8.78	0.0330	423.3271	0.0003

Table S2. Reproducibility of the extraction process based on UPLC-Q/TOF MS and  $^1\text{H}$  NMR.

UPLC-Q-TOF/MS								$^1\text{H}$ NMR		
Positive mode				Negative mode				NO.	$\delta^1\text{H}$ (ppm) and multiplicity	RSD (%)
NO.	RT (min)	$m/z$	RSD (%)	NO.	RT (min)	$m/z$	RSD (%)			
1	0.63	229.1522	2.3504	11	0.59	267.0722	11.4560	1	8.72 (dd)	10.5486
2	2.52	218.2117	6.0373	12	2.18	201.0223	8.5678	2	6.12 (d)	6.3553
3	2.60	260.2384	5.9340	13	4.82	265.1481	7.4356	3	4.465 (t)	7.9504
4	4.36	318.3002	4.3323	14	5.52	524.2751	3.4561	4	4.06 (s)	2.6738
5	5.20	302.3044	8.8344	15	6.01	540.3306	6.3427	5	2.99 (s)	9.5614
6	5.53	544.3409	11.4567	16	6.37	485.2828	9.1347	6	2.29 (d)	5.9702
7	5.94	496.3391	6.3527	17	7.04	568.3621	5.3467	7	2.07 (m)	3.2358
8	6.93	524.3715	4.3257	18	7.54	327.2371	6.8214	8	1.93 (s)	3.1454
9	7.55	637.3090	9.2347	19	7.71	303.2316	10.4672	9	1.88 (s)	5.7524
10	8.79	621.3092	5.2305	20	8.78	423.3271	8.3567	10	0.82 (m)	8.9037