

Figure S1. Ultra-high performance liquid chromatography-quadrupole time-of-flight mass spectrometry fingerprint of *Melastoma dodecandrum* Lour. in the negative mode.

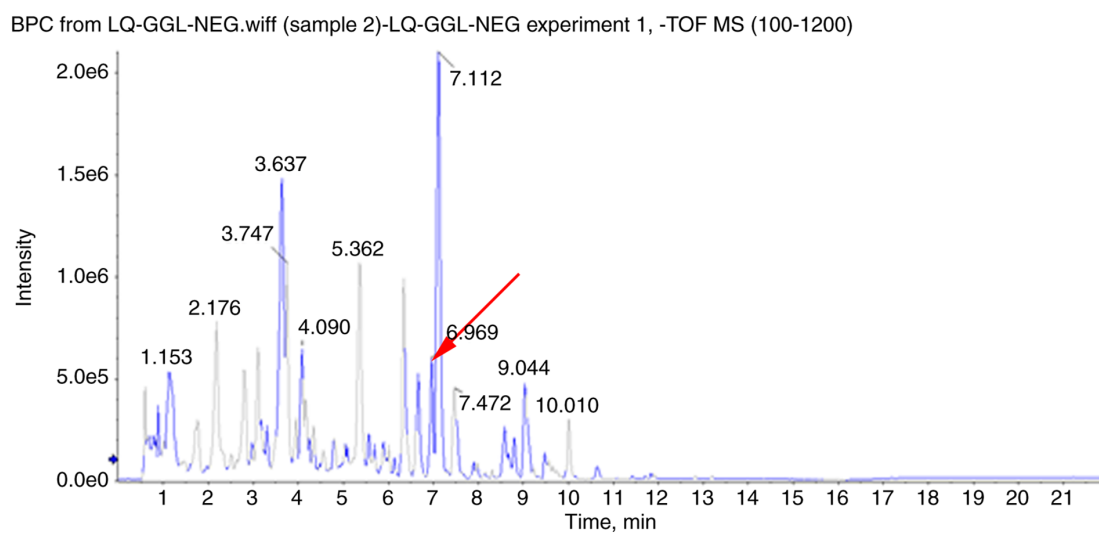


Figure S2. Ultra-high performance liquid chromatography-quadrupole time-of-flight mass spectrometry fingerprint of *Melastoma dodecandrum* Lour. in the positive mode.

BPC from LQ-GGL-POS.wiff (sample 1)-LQ-GGL-POS experiment 1, +TOF MS (100-1200)

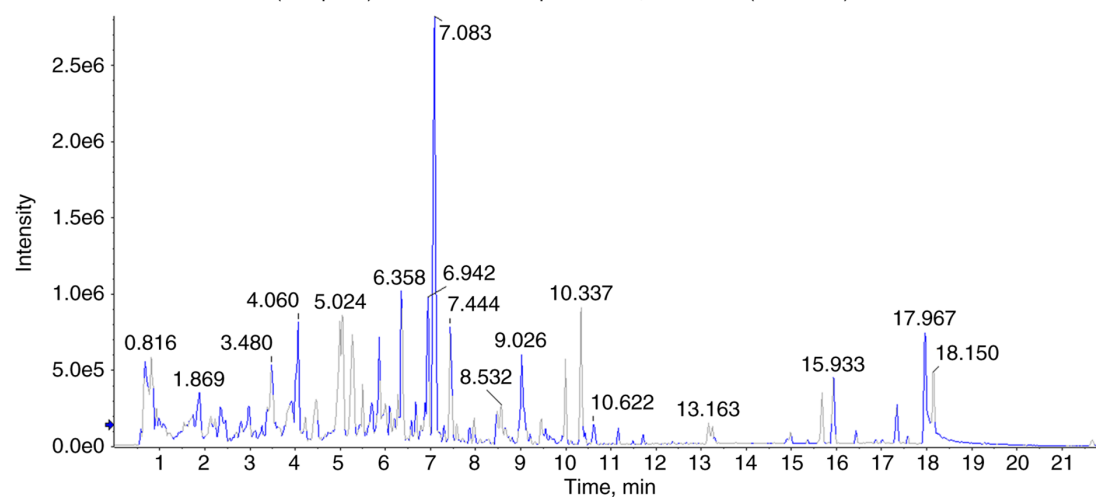


Table SI. Ultra-high performance liquid chromatography-quadrupole time-of-flight mass spectrometry detection of the chemical composition of *Melastoma dodecandrum* Lour in the negative mode.

Compound	Fragments, m/z	Retention time, min
2-Isopropylmalic acid	175.0614	3.00
Azelaic acid	187.0979	6.38
Caffeic acid	179.0357	3.42
Dodecanedioic acid	229.1452	9.25
D-(+)-Mannose	179.0557	0.68
p-Coumaric acid	163.0404	4.53
Sebacic acid	201.1136	7.39
Traumatic acid	227.1292	8.86
Undecanedioic acid	215.1292	8.45
Gingerglycolipid B	723.3808	12.36
Eupatilin	343.1548	10.85
Isoferulic acid	193.0514	5.22
Naringenin	271.0604	8.17
Citric acid	191.0204	0.89
Corilagin	633.0741	2.18
Quercetin	301.0351	7.31
Aurantio-Obtusin	329.0305	7.52
Narcissoside	623.1622	5.95
Gallic acid	169.0147	1.15
Vitexin	431.0980	5.36
Esculetin	177.0191	3.33
Astragalin	447.0926	6.01
Orientin	447.0926	4.82
Shikimic acid	173.0455	0.78
Hyperin	463.0874	5.50
Pedunculoside	695.4015	8.66
Cryptochlorogenic acid	353.0875	3.25

Table SII. Ultra-high performance liquid chromatography-quadrupole time-of-flight mass spectrometry detection of the chemical composition of *Melastoma dodecandrum* Lour in the positive mode.

Compound	Fragments, m/z	Retention time, min
5'-Methylthioadenosine	298.0968	2.36
5-Hydroxymethylfurfural	127.0389	1.70
Ellagic acid	303.0135	2.13
L-Tryptophan	205.0971	2.41
L-Tyrosine	182.0812	0.92
Syringaldehyde	183.0648	4.77
Deacetyl asperulosidic acid methyl ester	427.1212	2.43
Hederagenin	495.3430	12.77
Luteoloside	449.1068	5.91
Vitexin	433.1134	5.27
Syringa vulgaris	395.1310	3.11
L-Valine	118.0858	0.89
Cinnamic acid	149.021	1.65
Proline	116.0704	0.70
Adenosine	268.1047	0.92
Rutin	611.1610	5.23
Phenprobamate	166.0865	1.66
Orientin	449.1085	4.67
Ligustilide	191.1066	4.45
Betulonicacid	455.3507	12.77
Muscone	239.2367	15.93