SUPPLEMENTARY MATERIALS

Table S1. The MRM parameters and MS/MS transitions for analysis of phenolic compounds and triterpenoids

Compounds	Retention time (min)	Precursor ion (m/z)	Product ion (m/z)	Fragmentor (V)	Collision energy (V)
Catechin	1.52	291.1	139	90	7
EGCG	2.46	459.0	139	90	18
Myricetin glucoside	4.06	481.1	319	90	7
Myricetin rhamnoside	5.49	465.1	319	80	5
Quercetin glucoside	6.02	465.1	303	100	7
Quercetin arabinoside	6.79	435.1	303	90	2
Quercetin rhamnoside	6.97	449.0	303	80	5
Quercetin	8.30	303.1	153	170	30
Gallic acid	1.15	168.9	125	90	10
3,4-DHBA	1.77	153.0	109	80	10
p-coumaric acid	5.57	162.9	119	85	10
Madecassic acid	3.68	469.3	189.1	140	27
Asiatic acid	4.61	453.3	201.1	130	25
Hederagenin	7.08	455.3	189.1	120	25
Maslinic acid	8.53	455.3	203.1	120	25
Corosolic acid	8.93	455.3	205.1	120	20
Betulin	11.71	425.3	191.1	130	25
Betulinic acid	12.66	439.3	137.1	130	25
Oleanolic acid	13.67	439.3	203.1	130	25
Ursolic acid	13.98	439.3	203.1	130	25

Table S2. Regression equations and coefficients, linear ranges, limit of detection, limit of quantification, and recovery of the analytes

| Analyte	Regression equation	R^2	Range (mg/L)	LOD (µg/L)	LOQ (µg/L)	Average recovery (%)
Catechin	y = 34.5x - 694	0.9987	0.05-5.0	1.5	4.5	102.1 ± 8.1
EGCG	y = 27.0x - 4010	0.9961	0.01-0.5	3.5	10.5	104.0 ± 7.5
Myricetin glucoside	y = 70.6x - 5540	0.9973	0.01-0.5	2.0	6.0	105.0 ± 8.2
Myricetin rhamnoside	y = 52.6x - 1609	0.9981	0.25-5.0	2.0	6.0	100.5 ± 6.2
Quercetin glucoside	y = 71.3x - 140	0.9997	0.01-0.5	1.5	4.5	106.7 ± 7.4
Quercetin arabinoside	y = 59.5x + 2056	0.9992	0.1-2.5	2.0	6.0	104.4 ± 3.8
Quercetin rhamnoside	y = 42.8x - 2243	0.9988	0.1-0.5	1.5	4.5	102.9 ± 7.4
Quercetin	y = 3.0x - 208	0.9973	0.1-0.5	5.0	15.0	79.0 ± 8.0
Gallic acid	y = 25.3x - 337	0.9992	0.05-5.0	10.0	30.0	79.2 ± 7.2
3,4-DHBA	y = 29.9x + 2	0.9970	0.05-1.0	2.0	6.0	102.1 ± 8.0
p-coumaric acid	y = 147.3x + 3610	0.9957	0.05-1.0	1.0	3.0	101.5 ± 7.1
Madecassic acid	y = 88.2x + 70	0.9995	0.01-0.2	1.5	4.5	84.0 ± 4.0
Asiatic acid	y = 334.6x – 277.3	0.9997	0.01-0.5	2.2	6.6	102.3 ± 1.5
Hederagenin	y = 612.4x - 1418	0.9996	0.01-0.5	0.8	2.4	98.7 ± 3.5
Maslinic acid	y = 283.2x + 476.7	0.9998	0.01-0.5	1.4	4.2	99.3 ± 1.7
Corosolic acid	y = 681.3x - 1896	0.9997	0.01-0.5	2.8	8.4	101.0 ± 1.7
Betulin	y = 47.32x – 230.7	0.9986	0.01-0.5	1.1	3.3	102.1 ± 2.2
Betulinic acid	y = 13.3x + 237	0.9948	0.1-1.0	9.1	27.3	101.3 ± 2.1
Oleanolic acid	y = 758.8x – 2795	0.9991	0.01-1.0	1.4	4.2	100.0 ± 2.6
Ursolic acid	y = 729.9x - 3648	0.9989	0.01-1.0	1.3	3.9	99.7 ± 3.1
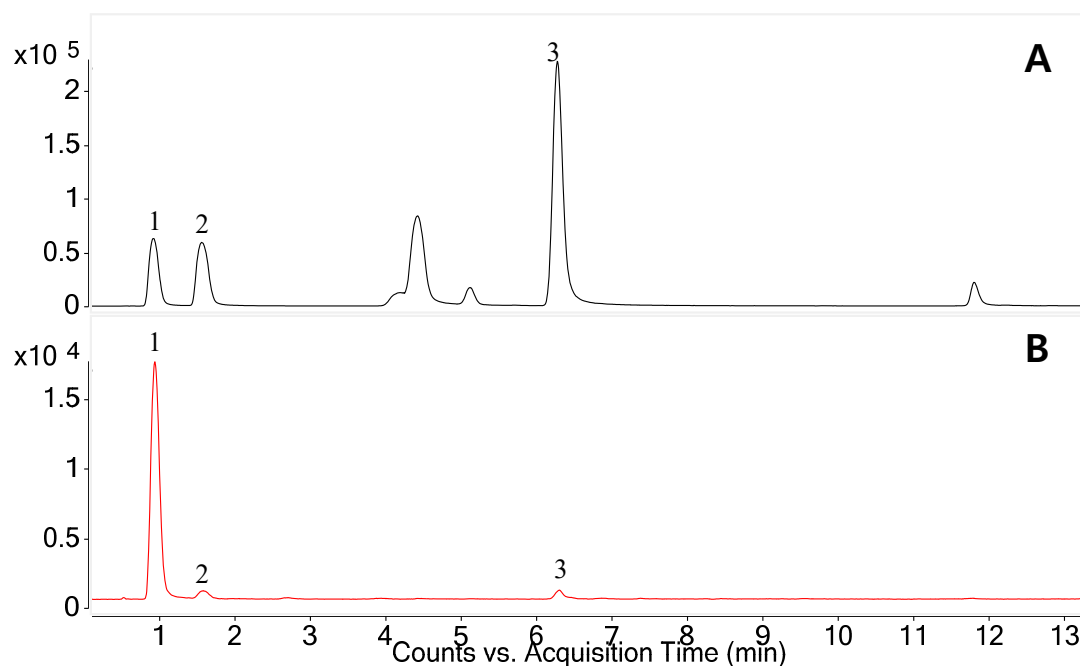
Figure S1. The MRM chromatogram of detected phenolic acids in *Syzygium formosum* leaves (A: Mixed standard, B: Sample; *1- Gallic acid, 2-3,4-dihydrobenzoic acid, 3-p-coumaric acid)*
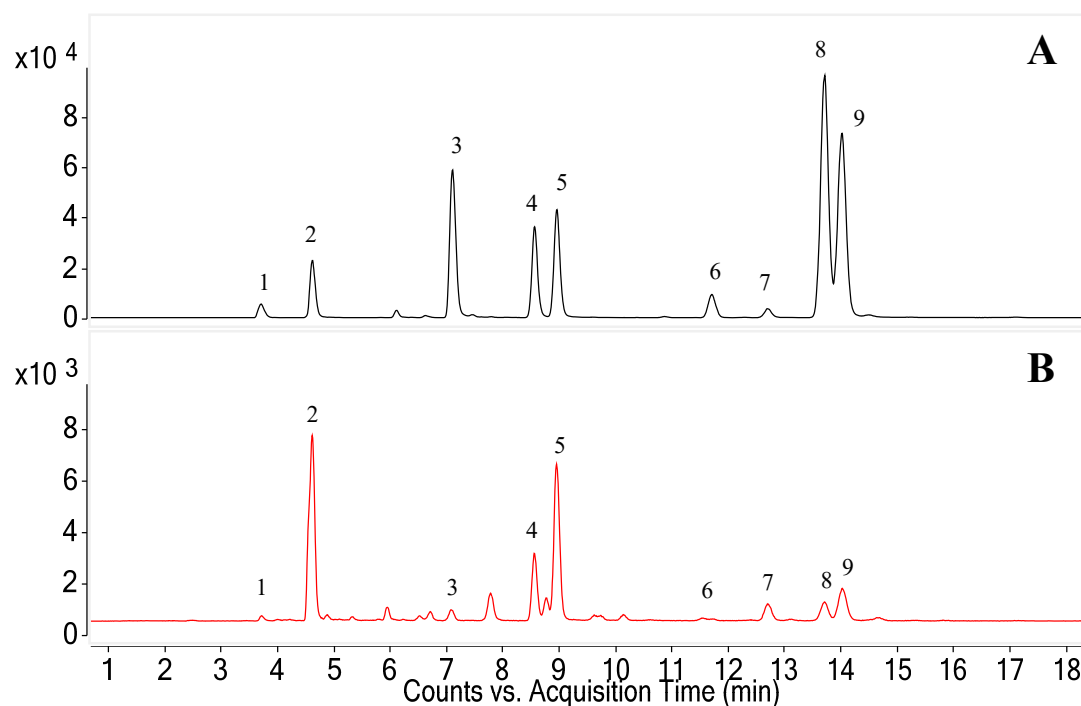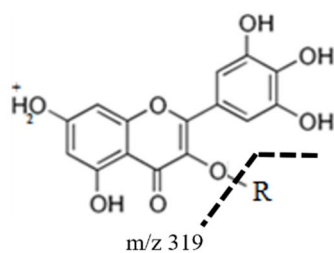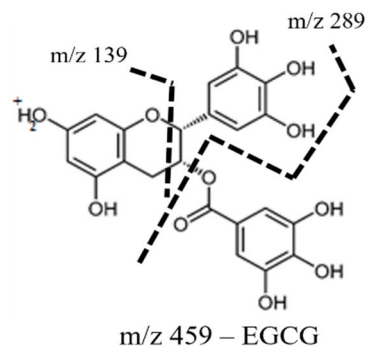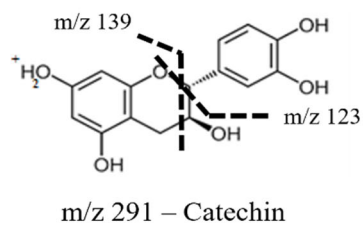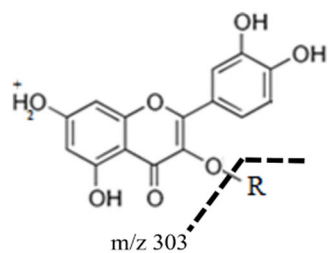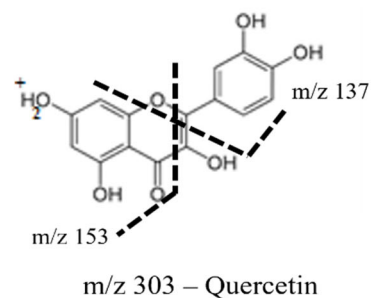

Figure S2. The MRM chromatogram of detected triterpenoids in *Syzygium formosum* leaves (A: Mixed standard, B: Sample; *1-Madecassic acid, 2- Asiatic acid, 3- Hederagenin, 4-Maslinic acid, 5-Corosolic acid, 6- Betulin, 7-Betulinic acid, 8-Oleanolic acid, 9- Ursolic acid)*
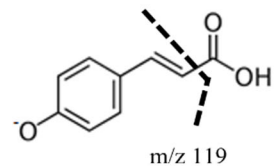
A)

m/z 139

m/z 123

m/z 291 – Catechin

m/z 289

m/z 139

m/z 459 – EGCG

m/z 319

m/z 481 (R- Glu) – Myricetin glucoside
m/z 465 (R- Rha) – Myricetin rhamnoside

m/z 137

m/z 153

m/z 303 – Quercetin

m/z 303

m/z 465 (R- Glu) – Quercetin glucoside
m/z 435 (R- Ara) – Quercetin arabinoside
m/z 449 (R- Rha) – Quercetin rhamnoside

m/z 125

m/z 169 – Gallic acid

m/z 109

m/z 153 – 3,4-dihydrobenzoic acid

m/z 119

m/z 163 – p-coumaric acid

B)

m/z 191.1

- 2H →

m/z 189.1

+ 2H →

m/z 233.1

m/z 235.1

- CH₃ ↑

- CH₃ ↑

m/z 206.1

m/z 455.3 Hederagenin

- COOH →

m/z 248.1

- C₂H₂ →

m/z 203.1

m/z 177.1

- H₂O ↑

- 2H₂O →

- R₄ →

- CH₃ →

- 2H →

m/z 469.3 Madecassic acid
m/z 453.3 Asiatic acid

m/z 204.1

m/z 189.1

m/z 187.1

R₁	R₂	R3	R4	
-H	-CH₃	-OH	-OH	Madecassic acid
-H	-CH₃	-OH	-H	Asiatic acid
-CH₃	-H	-H	-H	Hederagenin

Figure S3. (Continued)

C)

R₁   R₂   R3
-CH₃ -H   -H   Oleanolic acid   m/z 439.3
-H   -CH₃ -H   Ursolic acid   m/z 439.3
-CH₃ -H   -OH   Maslinic acid   m/z 455.3
-H   -CH₃ -OH   Corosolic acid   m/z 455.3

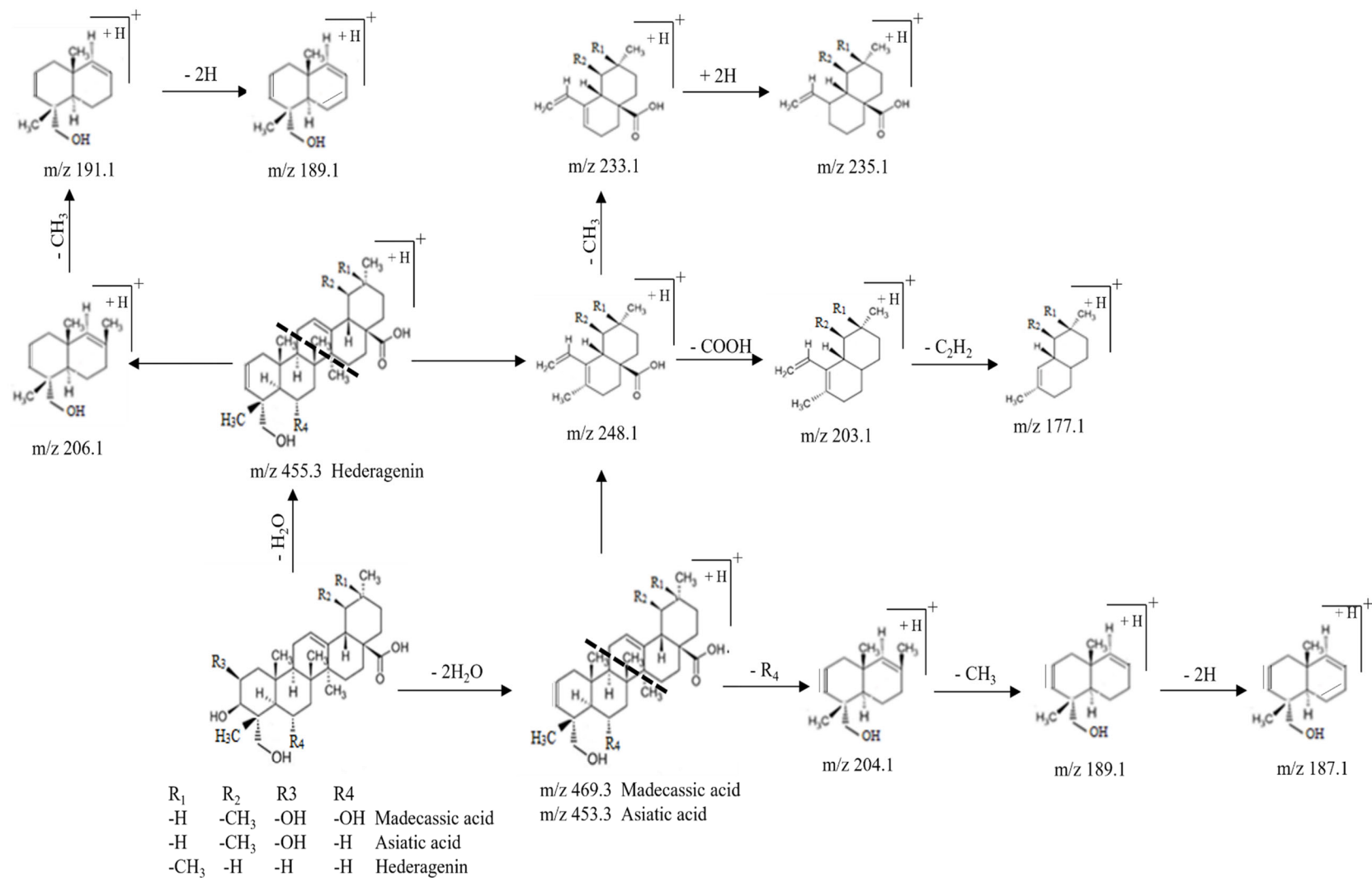R= -CH₂OH   Betulin   m/z 425.3
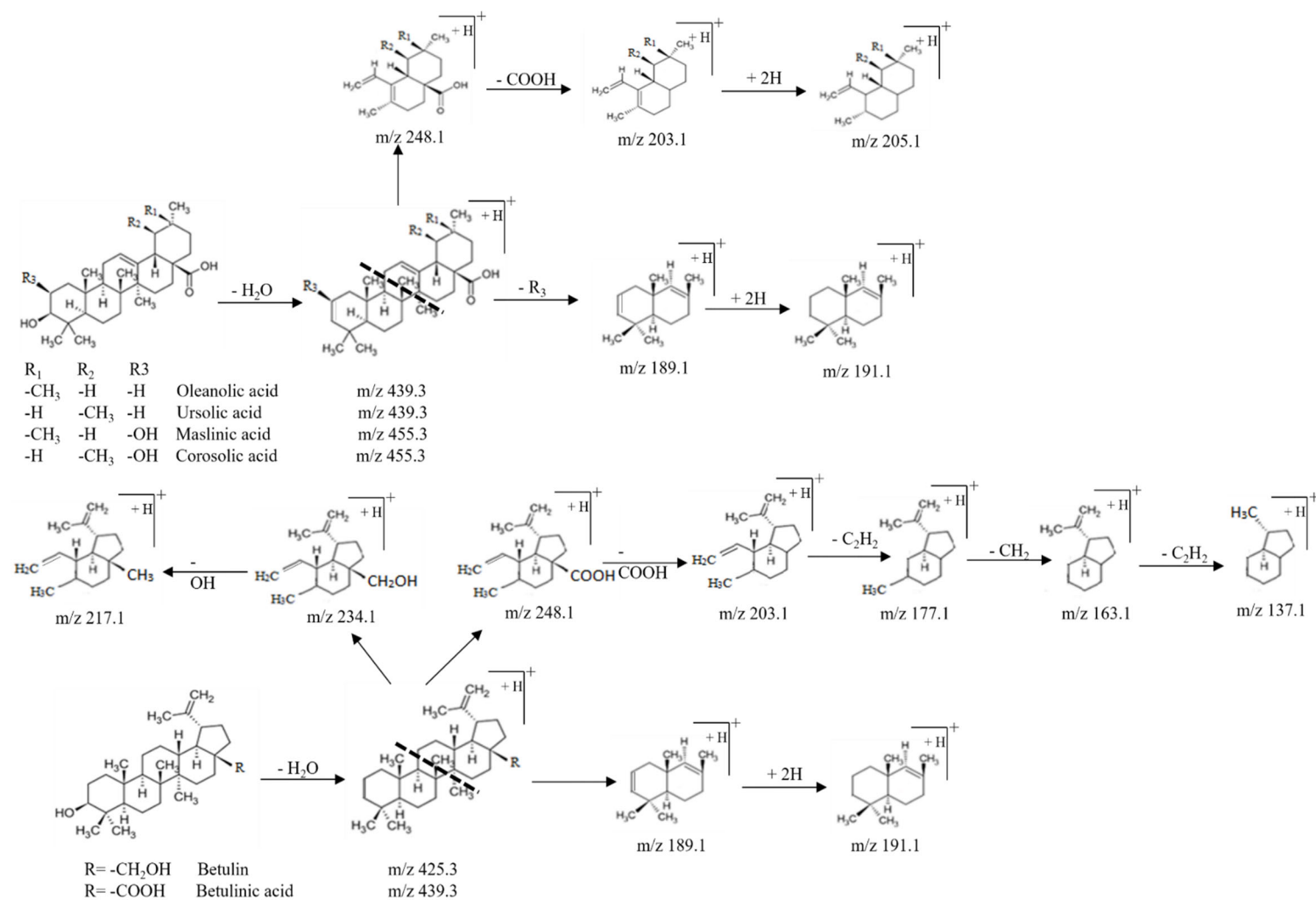R= -COOH   Betulinic acid   m/z 439.3

Figure S3. (Continued)

Figure S3. Proposed fragmentation of phenolic compounds (A) and triterpenoids (B and C) in *Syzygium formosum* leaves