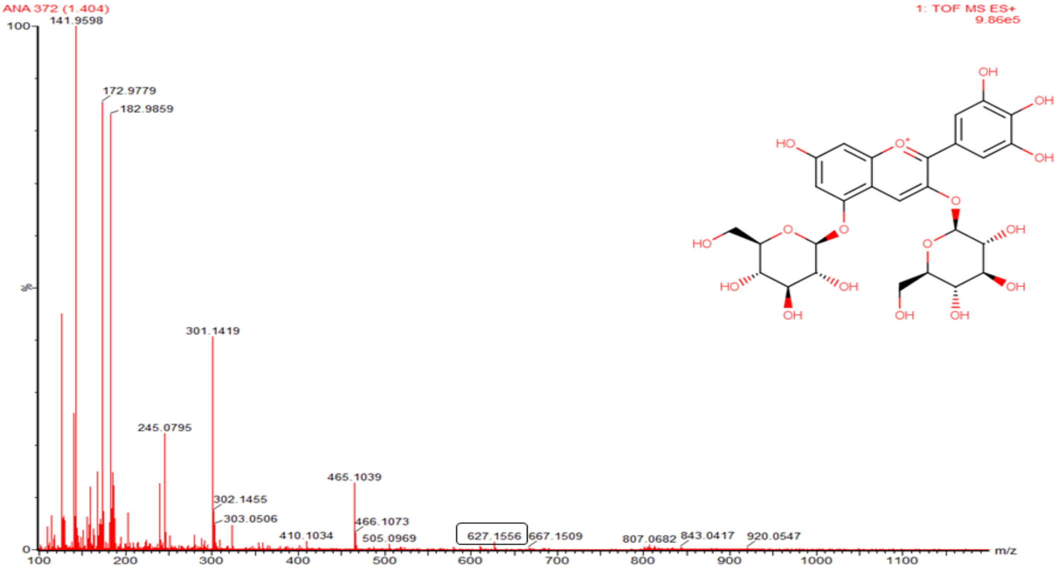
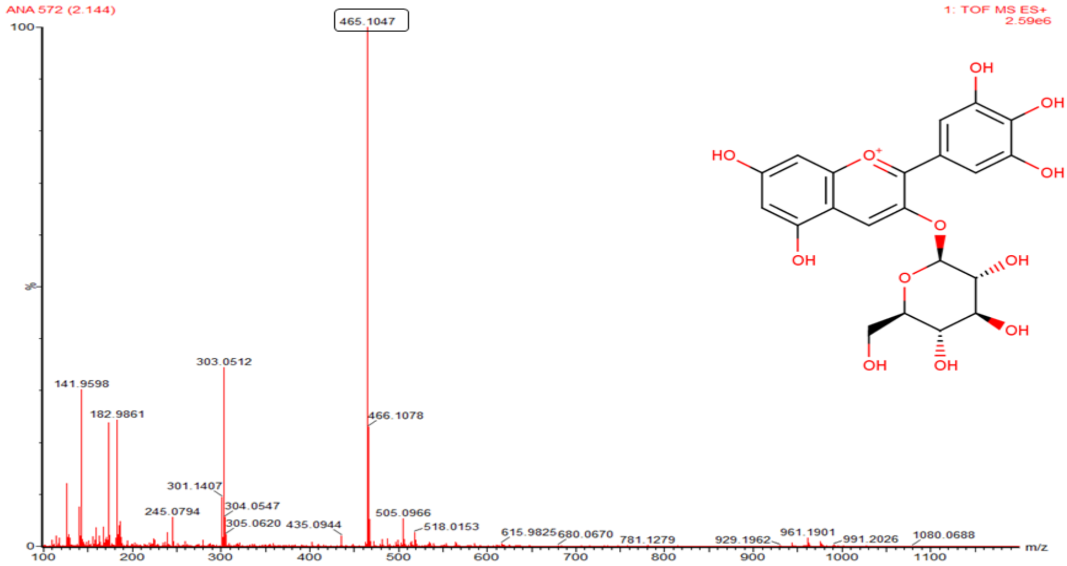
Table S1: Mass spectra information of the eleven anthocyanins present in myrtle berries.

Anthocyanins present in myrtle berries	**Molecular formula**	**Theoretical mass (*m*/*z*)**	**Measured mass (*m*/*z*)**
Delphinidin 3,5-*O*-diglucoside	$C_{27}H_{31}O_{17}$	627.1561	627.1556
Delphinidin 3-*O*-glucoside	$C_{21}H_{21}O_{12}$	465.1033	465.1047
Cyanidin 3-*O*-galactoside	$C_{21}H_{21}O_{11}$	449.1084	449.1089
Cyanidin 3-*O*-glucoside	$C_{21}H_{21}O_{11}$	449.1084	449.1089
Cyanidin 3-*O*-arabinoside	$C_{20}H_{19}O_{10}$	419.0978	419.0979
Petunidin 3-*O*-glucoside	$C_{22}H_{23}O_{12}$	479.1190	479.1195
Delphinidin 3-*O*-arabinoside	$C_{20}H_{19}O_{11}$	435.0927	435.0931
Peonidin 3-*O*-glucoside	$C_{22}H_{23}O_{11}$	463.1240	463.1249
Malvidin 3-*O*-glucoside	$C_{23}H_{25}O_{12}$	493.1346	493.1385
Petunidin 3-*O*-arabinoside	$C_{21}H_{21}O_{11}$	449.1084	449.1101
Malvidin 3-*O*-arabinoside	$C_{22}H_{23}O_{11}$	463.1240	463.1238

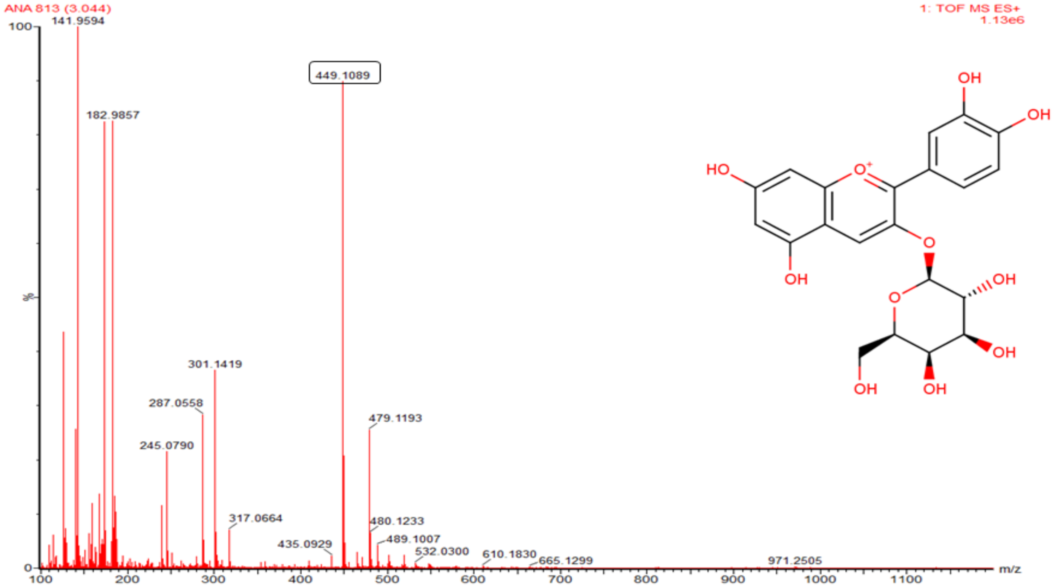
(a)



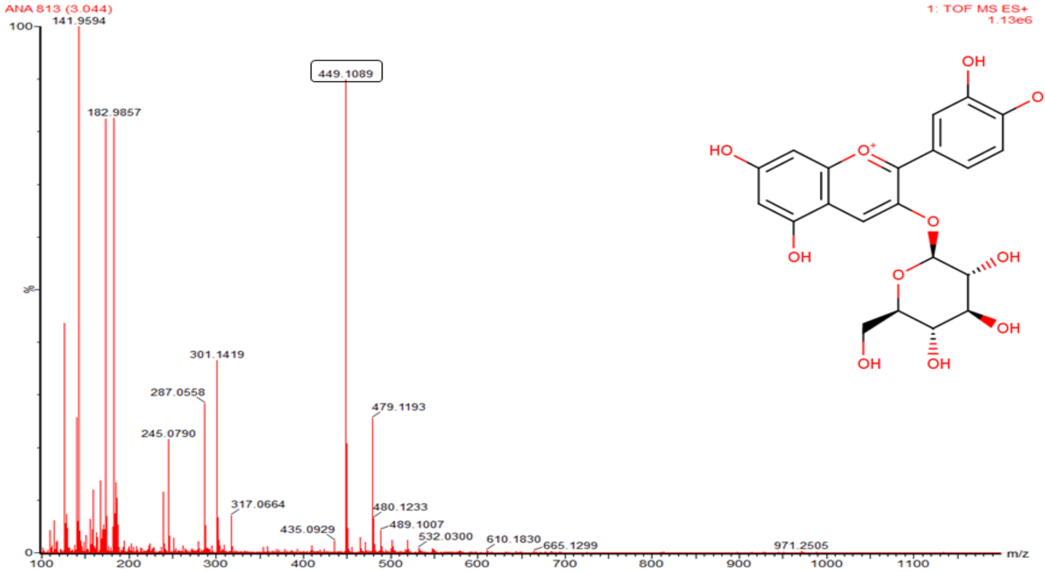
(b)


ANA 572 (2.144)
1: TOF MS ES+
2.59e6
465.1047
141.9598
182.9861
303.0512
301.1407
245.0794
304.0547
305.0620
435.0944
466.1078
505.0966
518.0153
615.9825
680.0670
781.1279
929.1962
961.1901
991.2026
1080.0688
100
%
0
m/z
HO
O+
OH
OH
OH
O
O
OH
OH
OH
OH
OH

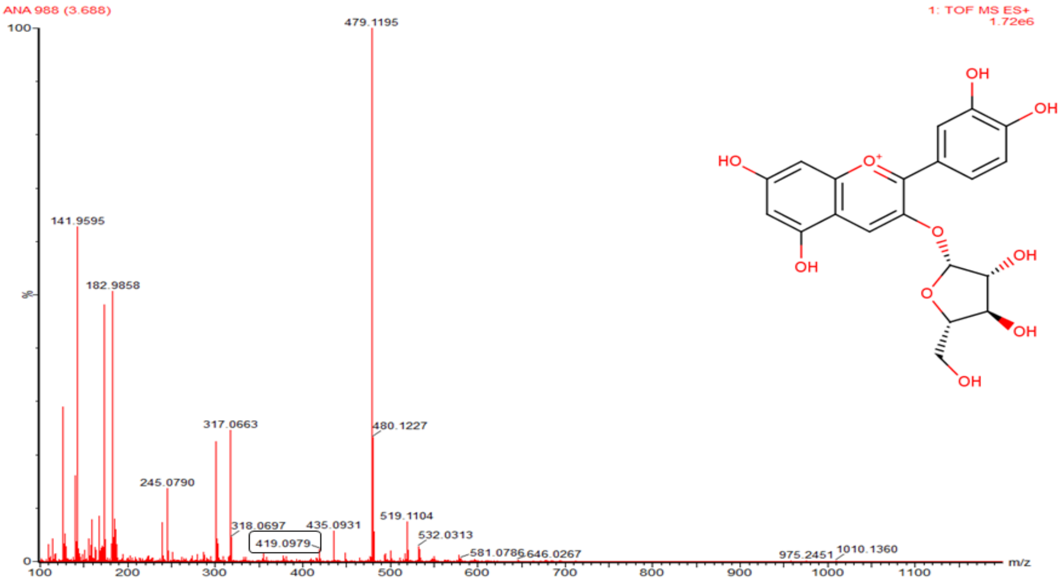
(c)


ANA 813 (3.044)
1: TOF MS ES+
1.13e6
141.9594
449.1089
182.9857
301.1419
287.0558
245.0790
479.1193
317.0664
480.1233
435.0929
489.1007
532.0300
610.1830
665.1299
971.2505
100
%
0
m/z
HO
O+
OH
OH
OH
O
O
OH
OH
OH
OH

(d)

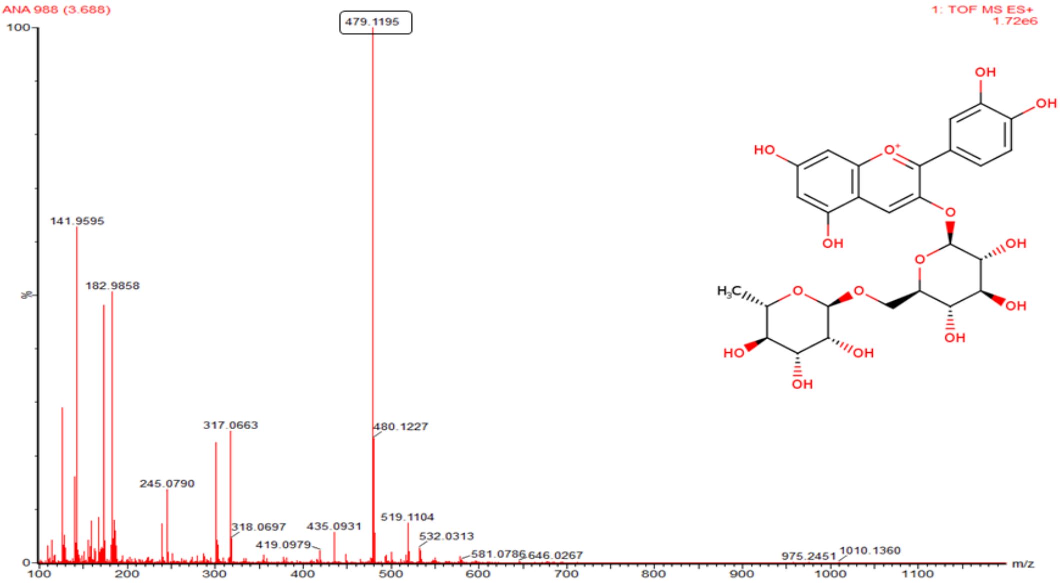

ANA 813 (3.044)
1: TOF MS ES+
1.13e6
141.9594
449.1089
182.9857
301.1419
287.0558
245.0790
479.1193
317.0664
480.1233
435.0929
489.1007
532.0300
610.1830
665.1299
971.2505
100
%
0
m/z
HO
O+
OH
OH
OH
O
O
OH
OH
OH
OH

(e)



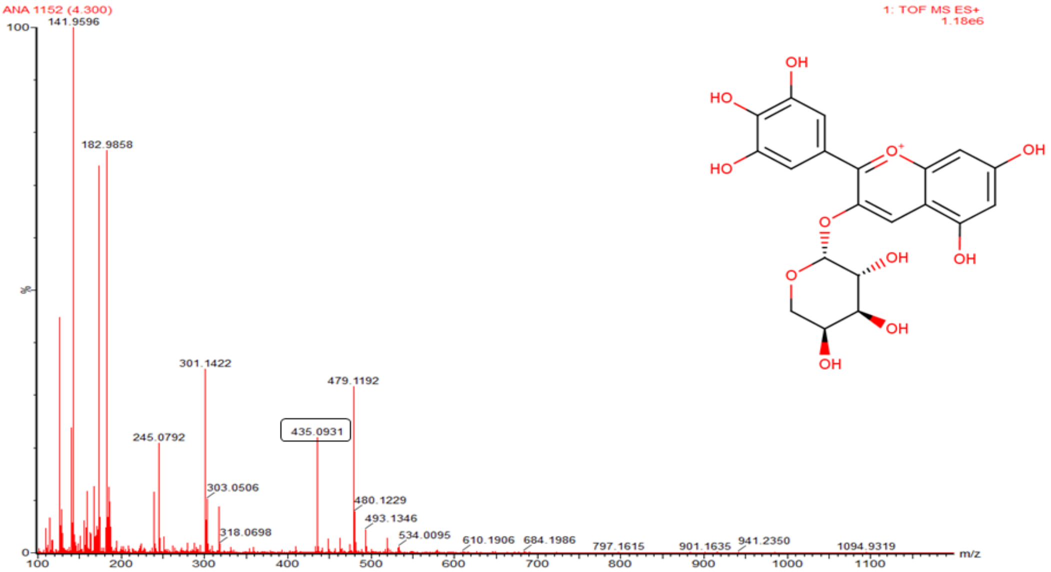
ANA 988 (3.688)
1: TOF MS ES+
1.72e6
100
%
0
479.1195
141.9595
182.9858
317.0663
480.1227
245.0790
519.1104
318.0697
435.0931
419.0979
532.0313
581.0786
646.0267
975.2451
1010.1360
100
200
300
400
500
600
700
800
900
1000
1100
m/z
OH
OH
HO
O+
O
OH
OH
OH
O
OH

(f)



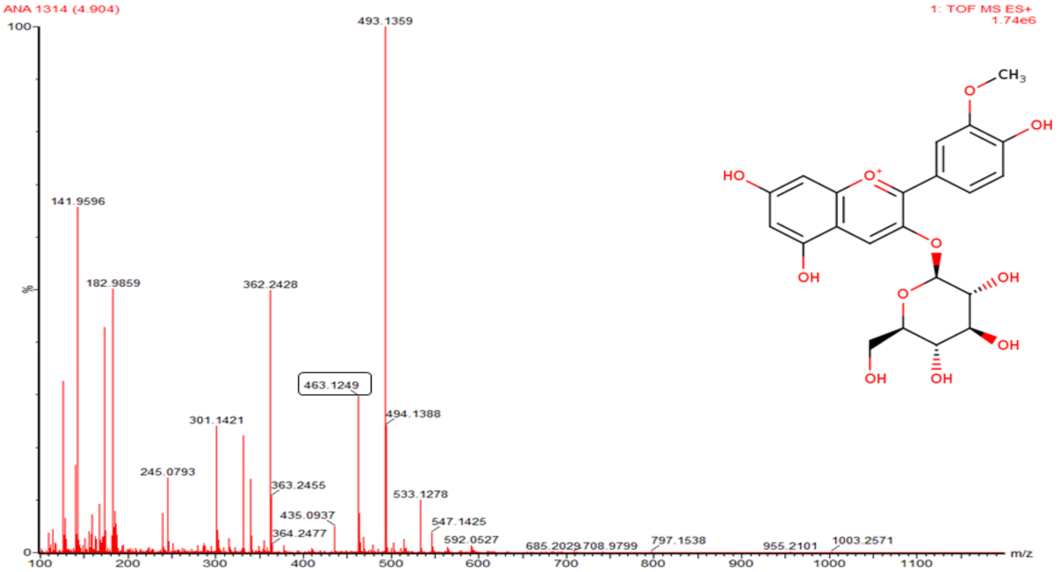
ANA 988 (3.688)
1: TOF MS ES+
1.72e6
100
%
0
479.1195
141.9595
182.9858
317.0663
480.1227
245.0790
519.1104
318.0697
435.0931
419.0979
532.0313
581.0786
646.0267
975.2451
1010.1360
100
200
300
400
500
600
700
800
900
1000
1100
m/z
OH
OH
HO
O+
O
OH
OH
O
O
H_3C
O
OH
OH
HO
OH

(g)

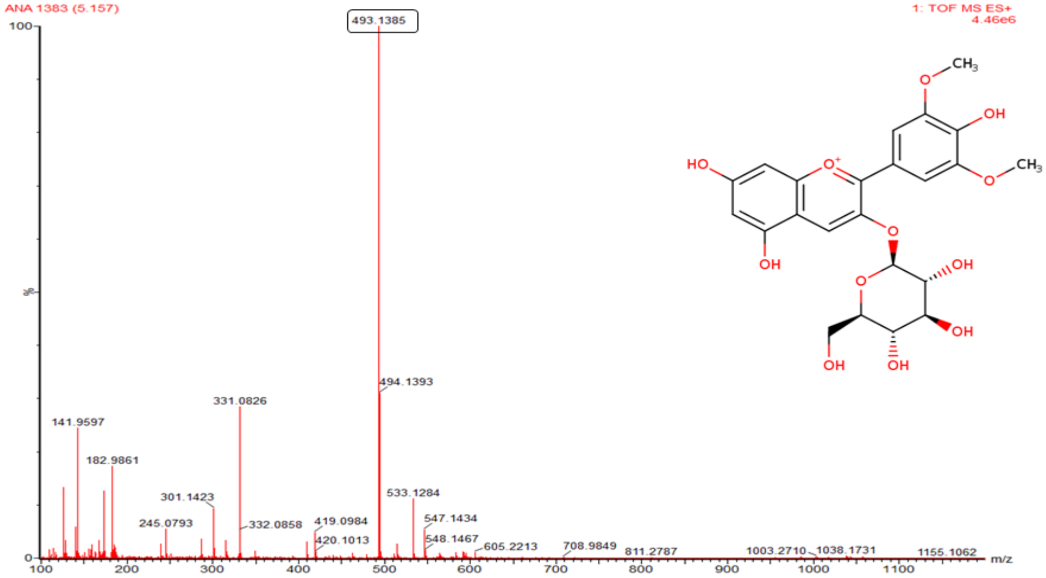


ANA 1152 (4.300)
1: TOF MS ES+
1.18e6
100
%
0
141.9596
182.9858
301.1422
479.1192
435.0931
245.0792
303.0506
480.1229
493.1346
318.0698
534.0095
610.1906
684.1986
797.1615
901.1635
941.2350
1094.9319
100
200
300
400
500
600
700
800
900
1000
1100
m/z
OH
HO
HO
O+
OH
OH
O
O
OH
OH
OH

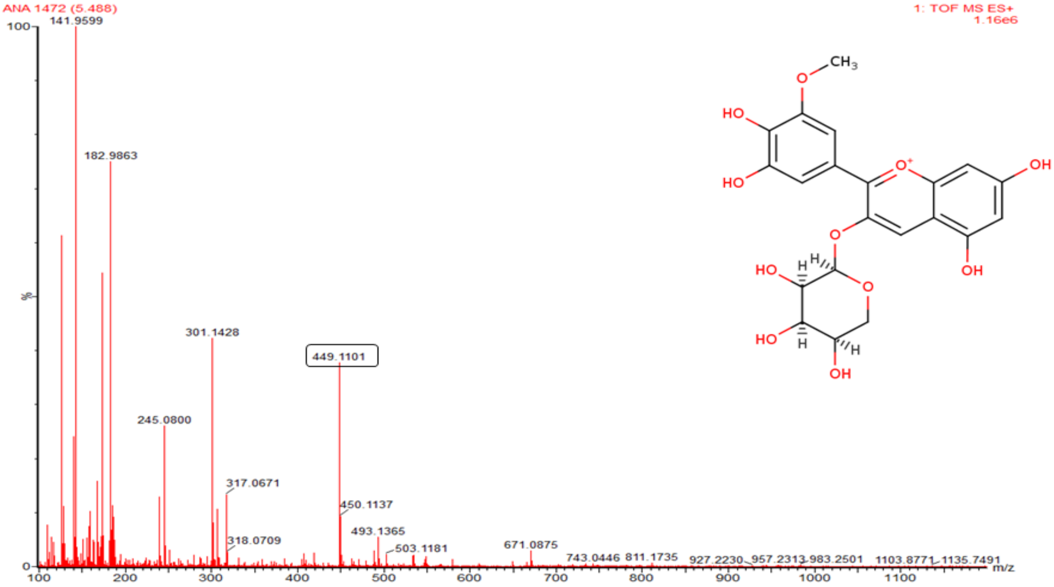
(h)


ANA 1314 (4.904)
1: TOF MS ES+
1.74e6
100
%
0
493.1359
141.9596
182.9859
362.2428
463.1249
494.1388
301.1421
245.0793
363.2455
533.1278
435.0937
547.1425
364.2477
592.0527
685.2029
708.9799
797.1538
955.2101
1003.2571
100
200
300
400
500
600
700
800
900
1000
1100
m/z
CH3
O
OH
HO
O+
OH
O
O
OH
OH
OH
OH

(i)


ANA 1383 (5.157)
1: TOF MS ES+
4.46e6
100
%
0
493.1385
494.1393
331.0826
141.9597
182.9861
301.1423
245.0793
332.0858
419.0984
420.1013
533.1284
547.1434
548.1467
605.2213
708.9849
811.2787
1003.2710
1038.1731
1155.1062
100
200
300
400
500
600
700
800
900
1000
1100
m/z
CH3
O
OH
O
CH3
HO
O+
OH
O
O
OH
OH
OH
OH

(j)


ANA 1472 (5.488)
1: TOF MS ES+
1.16e6
100
%
0
141.9599
182.9863
301.1428
449.1101
245.0800
317.0671
450.1137
318.0709
493.1365
503.1181
671.0875
743.0446
811.1735
927.2230
957.2313
983.2501
1103.8771
1135.7491
100
200
300
400
500
600
700
800
900
1000
1100
m/z
CH3
O
HO
HO
O+
OH
OH
O
HO
H
H
O
HO
H
H
OH

(k)

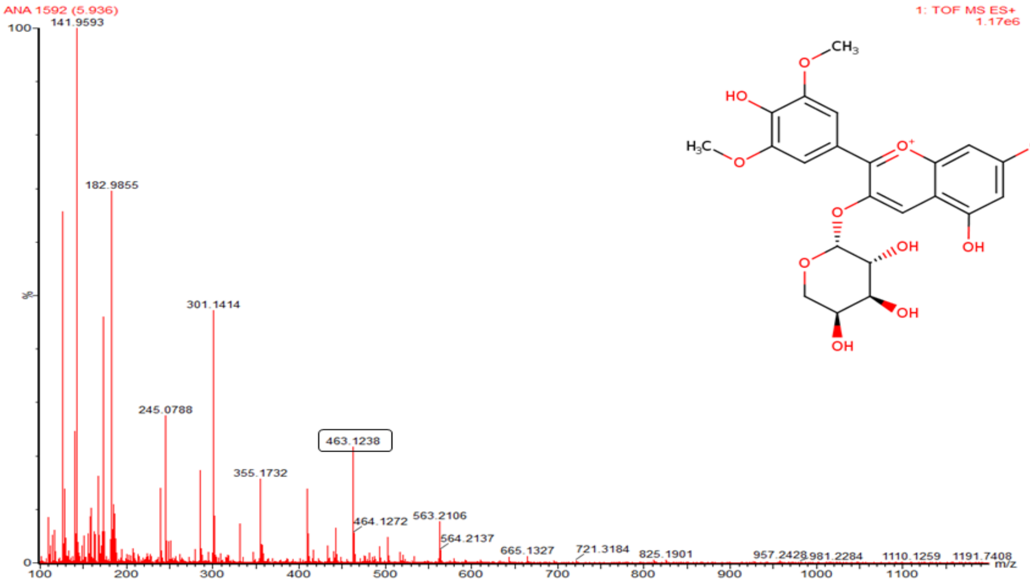


Figure S1: MS spectra and structure of the eleven anthocyanins identified in myrtle berries: (a) Delphinidin 3,5-*O*-diglucoside; (b) Delphinidin 3-*O*-glucoside; (c) Cyanidin 3-*O*-galactoside; (d) Cyanidin 3-*O*-glucoside; (e) Cyanidin 3-*O*-arabinoside; (f) Petunidin 3-*O*-glucoside; (g) Delphinidin 3-*O*-arabinoside; (h) Peonidin 3-*O*-glucoside; (i) Malvidin 3-*O*-glucoside; (j) Petunidin 3-*O*-arabinoside; (k) Malvidin 3-*O*-arabinoside.