S Table 2. Identification or characterization results of 15 selected metabolites in UPLC-QTOF-MS/MS analysis.

No.	RT (min)	Structures / name*	Formula	Exact mass	Parent ions	MS/MS
C1	20.18	Epoxy-octadecadienoic acid	$C_{18}H_{30}O_3$	294.2195	$[M+H]^+$ 295.2263	179.1407, 149.1327, 133.1013, 107.0837
					$[M-H]^-$ 293.2099	275.2034, 209.1170, 177.1295
C2	20.28	18:1 / Lyso-PC	$C_{26}H_{52}NO_7P$	521.3481	$[M+H]^+$ 522.3542	504.3393, 485.2601, 339.2883, 184.0737, 124.9992, 104.1065
					$[M+HCOOH-H]^-$ 566.3468	-
C3	19.73	16:0 / Lyso-PC	$C_{24}H_{50}NO_7P$	495.3325	$[M+H]^+$ 496.3388	184.0737, 124.9992, 104.1065
					$[M+HCOOH-H]^-$ 540.3293	-
C4	23.59	Masticadienonic acid	$C_{30}H_{46}O_3$	454.3447	$[M+H]^+$ 455.3511	437.3383, 419.3329, 381.3184, 355.2989, 311.2339, 251.1994, 113.0597
					$[M-H]^-$ 453.3354	409.3438, 355.2960
C5	19.33	Lyso-PC / 16:0	$C_{24}H_{50}NO_7P$	495.3325	$[M+H]^+$ 496.3388	184.0737, 124.9992, 104.1085
					$[M+HCOOH-H]^-$ 540.3293	-
C6	22.35	Camelledionol	$C_{29}H_{44}O_3$	440.3290	$[M+H]^+$ 441.3355	423.3229, 273.1879, 213.1623
					$[M-H]^-$ 439.3244	409.3107, 219.1388, 125.0979
C7	14.51	Trihydroxy-octadecenoic acid	$C_{18}H_{34}O_5$	330.2406	$[M+H]^+$ 331.2482	313.2370, 295.2263, 267.2346, 169.1243, 135.1202
					$[M-H]^-$ 329.2307	311.2196, 293.2099, 183.1367, 157.0879
C8	19.09	Dehydrated dyphylline-Glc-C16:0	$C_{32}H_{54}N_4O_{10}$	654.3840	$[M+H]^+$ 655.3870	537.3031, 515.3165, 313.2750
					$[M-H]^-$ 653.3713	415.1392, 397.1323, 255.2326, 253.0912, 235.0803, 179.0559, 161.0441, 116.9270, 101.0238
C9	17.59	Octadecanedioic acid	$C_{18}H_{34}O_4$	314.2457	$[M+H]^+$ 315.2537	235.2082, 139.1456, 125.1320
					$[M-H]^-$ 313.2385	295.2294, 223.2439, 197.1530, 113.0605
C10	19.88	Hydroxy-octadecatrienoic acid	$C_{18}H_{30}O_3$	294.2195	$[M+H]^+$ 295.2263	277.2205, 259.2044, 231.2117, 217.1964, 177.1661, 163.1482, 147.1180, 137.1351, 119.0863

					$[M-H]^-$ 293.2099	275.2000, 249.2199, 137.0936
C11	11.48	Hydroxycinnamaldehyde-Glc-Glc-Tetrahydroxyflavone	$C_{36}H_{36}O_{18}$	756.1902	$[M+H]^+$ 757.1896	447.0928, 309.0934, 285.0356, 147.0460, 119.0506
					$[M-H]^-$ 755.1750	591.1326, 429.0802, 283.0233, 151.0016, 145.0281, 117.0333
C12	2.20	Epigallocatechin	$C_{15}H_{14}O_7$	306.0740	$[M+H]^+$ 307.0821	289.0710, 163.0384, 151.0403, 139.0394, 121.0278
					$[M-H]^-$ 305.0661	261.0754, 219.0661, 179.0340, 165.0180, 137.0240, 125.0246, 109.0300
C13	6.86	Trihydroxyflavanone	$C_{15}H_{12}O_5$	272.0685	$[M+H]^+$ 273.0763	255.0636, 179.0339
					$[M-H]^-$ 271.0581	253.0488, 177.0177, 151.0041
C14	4.05	Epicatechin	$C_{15}H_{14}O_6$	290.0790	$[M+H]^+$ 291.0887	205.9647, 165.0564, 163.0384, 147.0435, 139.0394, 123.0441
					$[M-H]^-$ 289.0698	245.0802, 203.0705, 137.0240, 125.0246, 123.0452
C15	5.58	Ara-Rha-Tetrahydroxyflavone	$C_{26}H_{28}O_{14}$	564.1479	$[M+H]^+$ 565.1548	287.0567
					$[M-H]^-$ 563.1401	431.0930, 285.0421, 151.0016

Ara, arabinoside; Rha, rhamnoside; Glc, glucoside.

* Due to limits of UPLC-QTOF-MS/MS, locations of double bonds in fatty acids, the hydroxyls in flavonoids or the substituent groups could not be determined.