Supporting information

NOx, IL-1β, TNF-α, IL-6 inhibition effects and trypanocidal activity of banana (*Musa acuminata*) bracts and flowers: UPLC-HRESI-MS detection of phenylpropanoid sucrose esters.

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Table S1. Chemical constituents of the flower fractions.

FDCM						
tR	**BPI (m/z)**	**Mass calculated (m/z)**	**Molecular formula**	**Fragment**	Proposed structure	**Ref.**
6.66	613.1731 $[M-H]^-$	613.1769	$C_{27}H_{34}O_{16}$	571.1544	Tomenside A, mumeose G, mumeose S or mumeose H	[1-3]
6.99	613.1731 $[M-H]^-$	613.1769	$C_{27}H_{34}O_{16}$	571.1544	Tomenside A, mumeose G, mumeose S or mumeose H	[1-3]
7.32	655.1882 $[M-H]^-$	655.1874	$C_{29}H_{36}O_{17}$	613.1680, 595.1530, 571.1544, 553.1459, 467.1384, 425.1317, 349.0909, 187.0343, 163.0352, 145.0278	mumeose L or mumeose U	[2, 4]
7.58	655.1882 $[M-H]^-$	655.1874	$C_{29}H_{36}O_{17}$	613.1680, 595.1580, 571.1544, 553.1363, 535.1274, 467.1340, 425.1233, 391.0948, 383.1170, 349.0832, 307.0778, 289.0623, 217.0513, 205.0422, 187.0343, 163.0352, 145.0278, 119.0473	4,6,2',6'-O-tetraacetyl-3-O-cis-p-coumaroylsucrose or 4,6,2',6'-O-tetraacetyl-3-O-trans-p-coumaroylsucrose	[5]
7.94	697.1997 $[M-H]^-$	697.1980	$C_{31}H_{38}O_{18}$	655.1882, 637.1663, 467.1251, 349.0870, 163.0378, 145.0278	mumeose V or mumeose D	[2]
8.05	697.1997 $[M-H]^-$	697.1980	$C_{31}H_{38}O_{18}$	655.1852, 637.1766, 613.1680, 595.1580, 467.1340, 425.1486, 391.1028, 349.0870, 205.0480, 187.0343, 163.0352, 145.0278	Prunose I or mumeose N, or mumeose M or mumeose O	[4]
8.16	697.1997 $[M-H]^-$	697.1980	$C_{31}H_{38}O_{18}$	655.1882, 637.1663, 613.1680, 595.1580, 467.1340, 425.1567, 391.1028, 349.1176, 205.0480, 187.0371, 163.0352, 145.0254	Prunose I or mumeose N, or mumeose M or mumeose O	[4]
8.27	697.1997 $[M-H]^-$	697.1980	$C_{31}H_{38}O_{18}$	655.1882, 637.1714, 613.1730, 595.1580, 467.1517, 391.0988, 349.0870, 205.0480,	Prunose I or mumeose N, or mumeose M or mumeose O	[4]

				187.0371, 163.0352, 145.0278		
8.75	221.1191 $[M-H]^-$	221.1178	$C_{13}H_{18}O_3$	-	Alkylated phenol derivative	
10.80	277.1817 $[M-H]^-$	277.1804	$C_{17}H_{26}O_3$	-	NI	
11.02	265.1468 $[M-H]^-$	265.1440	$C_{15}H_{22}O_4$	-	NI	
14.22	279.2312 $[M-H]^-$	279.2324	$C_{18}H_{32}O_2$	-	Linoleic acid	[6]
14.69	255.2306 $[M-H]^-$	255.2324	$C_{16}H_{32}O_2$	-	1-hexadecylcarboxylic acid	[7]
14.80	281.2470 $[M-H]^-$	281.2481	$C_{18}H_{34}O_2$	-	Related to petroselinic acid	[8]
15.68	283.2680 $[M-H]^-$	283.2637	$C_{18}H_{36}O_2$	-	n-octadecanoic acid	[9]
FNBU						
0.49	191.0551 $[M-H]^-$	191.0561	$C_7H_{12}O_6$	-	Quinic acid	[10]
2.18	487.1465 $[M-H]^-$	487.1457	$C_{21}H_{28}O_{13}$	307.0706, 163.0431, 145.0352	3-O-*p*-coumaroylsucrose	[11]
2.37	487.1465 $[M-H]^-$	487.1457	$C_{21}H_{28}O_{13}$	341.0868, 179.0580	Cistanoside F	[12]
3.43	529.1561 $[M-H]^-$	529.1563	$C_{23}H_{30}O_{14}$	487.1449, 469.1057, 341.0905	Acetyl cistanoside F derivative	-
3.69	529.1561 $[M-H]^-$	529.1563	$C_{23}H_{30}O_{14}$	487.1330, 307.0742, 163.0405, 145.0352	mumeose A derivative	[13]
4.35	529.1561 $[M-H]^-$	529.1563	$C_{23}H_{30}O_{14}$	487.1330, 163.0352, 145.0254	mumeose A derivative	[13]
4.60	571.1593 $[M-H]^-$	571.1663	$C_{25}H_{32}O_{15}$	529.1467, 511.1470, 307.0814, 163.0405, 145.0352	mumeose B, P, or R	[2, 13]
5.15	571.1642 $[M-H]^-$	571.1663	$C_{25}H_{32}O_{15}$	529.1467, 511.1470, 307.0814, 163.0405, 145.0352	mumeose B, P, or R	[2, 13]
5.41	571.1671 $[M-H]^-$	571.1663	$C_{25}H_{32}O_{15}$	529.1514, 511.1470, 307.0778, 163.0352, 145.0354	mumeose B, P, or R	[2, 13]
5.70	571.1642 $[M-H]^-$	571.1663	$C_{25}H_{32}O_{15}$	529.1467, 511.1470, 307.0778, 163.0405, 145.0354	mumeose B, P, or R	[2, 13]
6.07	613.1731 $[M-H]^-$	613.1769	$C_{27}H_{34}O_{16}$	571.1592, 553.1507, 529.1467, 511.1423, 349.0909, 307.0814, 163.0378, 145.0278	Tomenside B derivative	[3]
6.18	613.1731	613.1769	$C_{27}H_{34}O_{16}$	571.1592, 553.1507,	Tomenside B derivative	[3]

	$[M-H]^-$			529.1467, 511.1423, 349.0909, 307.0814, 163.0378, 145.0278		
6.40	613.1731 $[M-H]^-$	613.1769	$C_{27}H_{34}O_{16}$	571.1592, 553.1507, 529.1467, 511.1423, 349.0909, 307.0814, 163.0378, 145.0278	Tomenside B derivative	[3]
6.66	613.1731 $[M-H]^-$	613.1769	$C_{27}H_{34}O_{16}$	571.1592, 553.1507, 529.1467, 511.1423, 349.0909, 307.0814, 163.0378, 145.0278	Tomenside B derivative	[3]
6.99	613.1731 $[M-H]^-$	613.1769	$C_{27}H_{34}O_{16}$	571.1592, 553.1507, 529.1467, 511.1423, 349.0909, 307.0814, 163.0378, 145.0278	Tomenside B derivative	[3]
7.32	655.1882 $[M-H]^-$	655.1874	$C_{29}H_{36}O_{17}$	613.1680, 595.1530, 571.1544, 553.1459, 467.1384, 425.1317, 349.0909, 205.0422, 187.0343, 163.0352, 145.0278	mumeose L or mumeose U	[2, 4]
7.58	655.1882 $[M-H]^-$	655.1874	$C_{29}H_{36}O_{17}$	613.1680, 595.1580, 571.1544, 553.1363, 535.1274, 467.1340, 425.1233, 391.0948, 383.1170, 349.0832, 307.0778, 289.0623, 217.0513, 205.0422, 187.0343, 163.0352, 145.0278, 119.0473	4,6,2',6'-O-tetraacetyl-3-O-cis-p-coumaroylsucrose or 4,6,2',6'-O-tetraacetyl-3-O-trans-p-coumaroylsucrose	[5]
8.75	221.1191 $[M-H]^-$	221.1178	$C_{13}H_{18}O_3$	-	Alkylated phenol derivative	-
11.80	1197.2529 $[2M+HCO_2]^-$	1197.2512	$C_{32}H_{24}O_{12}$	-	Procyanidin derivatives	-
12.60	637.1405 $[M+HCO_2]^-$	637.1405	$C_{27}H_{28}O_{15}$	-	Glycosylated flavonoid	-
13.45	455.3515 $[M-H]^-$	455.3525	$C_{30}H_{48}O_3$	-	Ursolic acid, betulenic acid or oleanolic acid	-
14.07	609.4099 $[M-H]^-$	609.4049	$C_{39}H_{56}O_5$	-	Betuline-3-caffeate or erythrodiol-3-caffeate	-

NI: not identified

Table S2. Chemical constituents of the bract fractions.

BDCM						
tR	**BPI (m/z)**	**Mass calculated (m/z)**	**Molecular formula**	**Fragment**	**Proposed structure**	**Ref.**
7.36	177.0550 $[M-H]^-$	177.0552	$C_{10}H_{10}O_3$	-	Coumaric acid methyl ester or 4-methoxycinnamic acid	[14]
10.69	721.3635 $[M+HCO_2]^-$ 675.3600 $[M-H]^-$	721.3647 675.3597	$C_{33}H_{56}O_{14}$	593.3170	Physakengose B	[15]
11.54	723.3801 $[M+HCO_2]^-$ 677.3730 $[M-H]^-$	723.3803 677.3690	$C_{33}H_{58}O_{14}$	595.2879, 397.1343	3'-O-isobutyryl-3-O-isovaleryl-2-O-lauroylsucrose or 2,3,4-tri(5-methylhexanoyl)-α-D-glucopyranosyl-β-D-fructofuranoside	[16]
11.76	559.3087 $[M+HCO_2]^-$	559.3060	$C_{34}H_{44}O_4$	-	Stilbene derivative	-
12.57	445.2352 $[M-H]^-$	445.2379	$C_{29}H_{34}O_4$	-	2-Arylbenzofuran derivative	-
13.78	447.2509 $[M-H]^-$	447.2535	$C_{29}H_{36}O_4$	-	Stilbene derivative	-
14.22	279.2312 $[M-H]^-$	279.2324	$C_{18}H_{32}O_2$	-	Linoleic acid derivative	[6]
14.66	255.2339 $[M-H]^-$	255.2324	$C_{16}H_{32}O_2$	-	Fatty acid	-
BNBU						
2.29	293.1223 $[M-H]^-$	293.1236	$C_{12}H_{22}O_8$	-	γ-methyl-δ-hydroxy-pentanoic acid β-D-glucopyranoside	-
3.76	431.1871 $[M-H]^-$	431.1858	$C_{27}H_{28}O_5$	-	NI	-
4.05	377.1757 $[M-H]^-$	377.1753	$C_{24}H_{26}O_4$	-	Benzofuran derivative	-
5.01	609.1482 $[M-H]^-$	609.1456	$C_{27}H_{30}O_{16}$	581.1510, 461.1089	Lucenin-2	[17]
7.87	431.1531 $[M-H]^-$	431.1553	$C_{19}H_{28}O_{11}$	349.0985, 331.0892, 113.0320	Diffusoside A or B	[18]
8.05	433.1710 $[M-H]^-$	433.1710	$C_{19}H_{30}O_{11}$	351.1140, 333.1045, 267.0643,	7-O-Ethylmorroniside	[19]

				249.0587, 113.0298, 101.0698		
8.31	435.1851 $[M-H]^-$	435.1866	$C_{19}H_{32}O_{11}$	375.1381, 351.1102, 333.1045, 249.0490, 223.0397, 175.0307, 113.0298, 101.0698	Iridoid derivative	-
8.75	221.1191 $[M-H]^-$	221.1178	$C_{13}H_{18}O_3$	-	Alkylated phenol derivative	-
13.23	447.2509 $[M-H]^-$	447.2535	$C_{29}H_{36}O_4$	-	Stilbene derivative	-

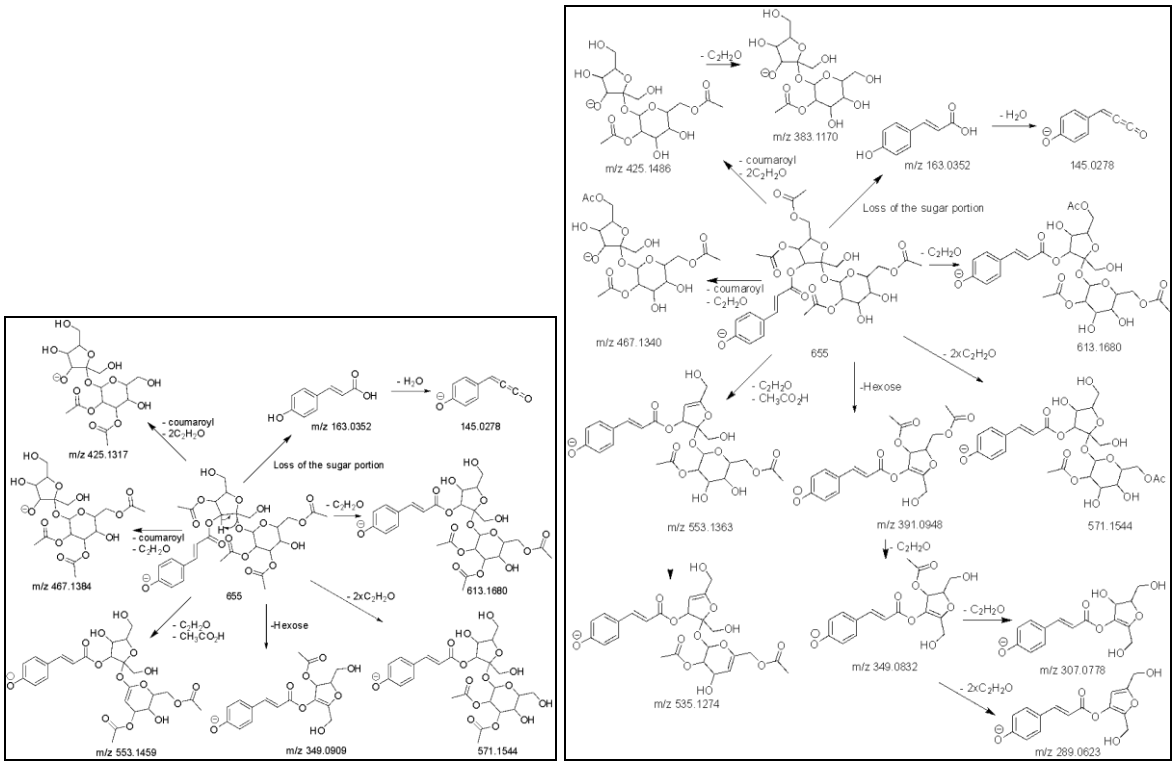

Figure S1. Fragmentation pattern of the metabolites m/z 655.1874 with retention times 7.32 min (left) and 7.58 min (right).

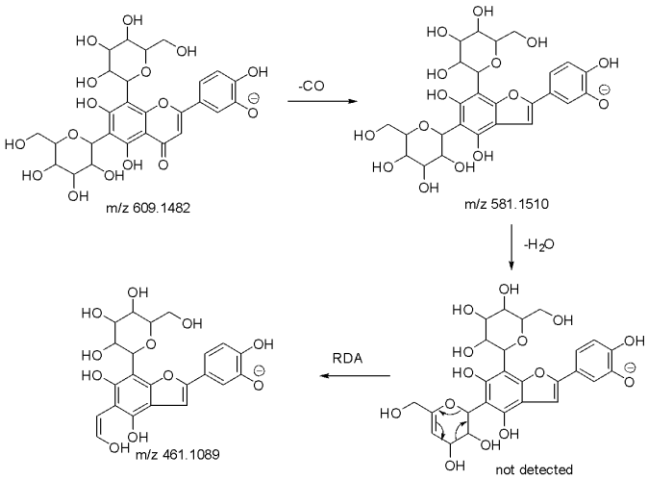

Figure S2. Fragmentation pattern of the metabolite m/z 609.1482.

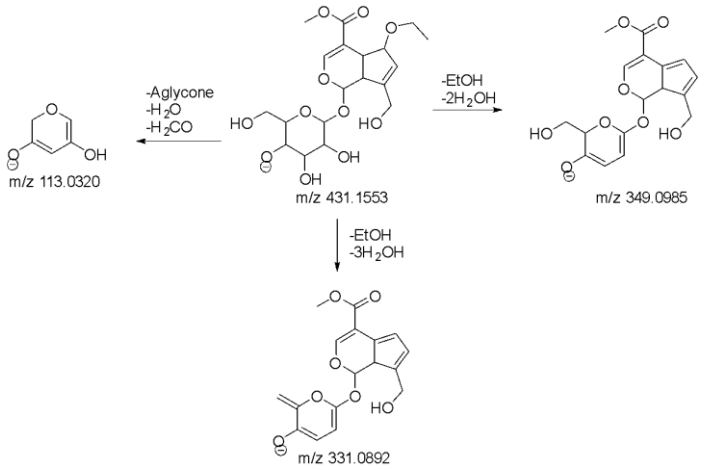

Figure S3. Fragmentation pattern of m/z 431.1553.

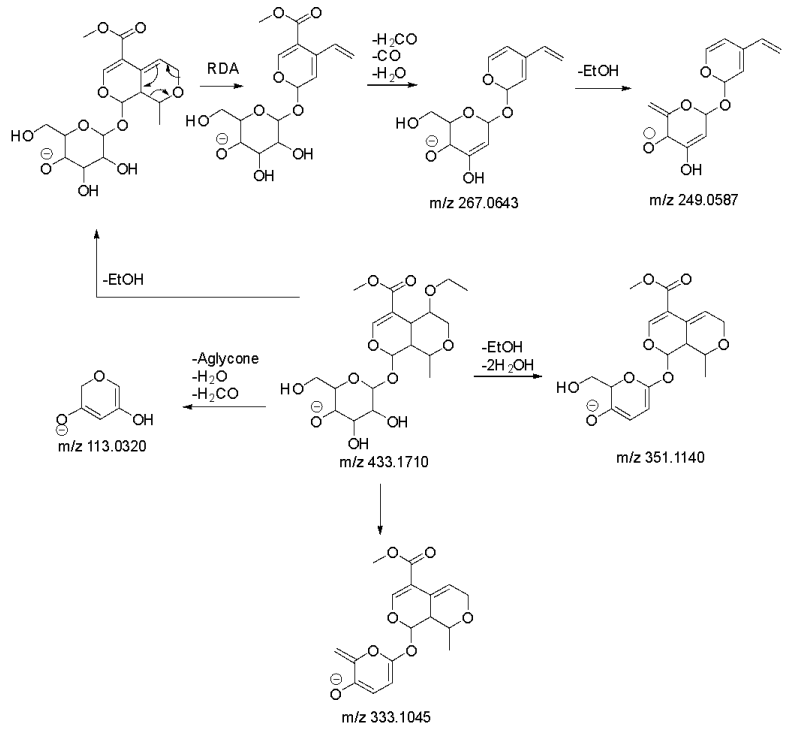

Figure S4. Fragmentation pattern of m/z 433.1710.

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