Table S3. Phytocannabinoid identification data, comprising compound identity, RT, proposed molecular formula, molecular weight, experimental m/z, calculated m/z, mass error (ppm), major product ions, and confidence level.

ID	Name	RT (min)	Proposed Formula	Molecular Weight	Experimental m/z	Calculated m/z	Δmass (ppm)	Main product ions	c. l.
C1	CBDOA	3.2	$C_{18}H_{22}O_4$	302.1520	301.1448	301.1445	0.7	301.1444; 283.1340; 257.1546; 189.0913; 135.0440; 123.0440	2
C2	CBCOA	7.7	$C_{18}H_{22}O_4$	302.1521	301.1448	301.1445	0.9	301.1444; 283.1340; 257.1546; 187.0756; 135.0440; 123.0440	2
C3	CBGOA	4.0	$C_{18}H_{24}O_4$	304.1677	303.1605	303.1602	0.9	303.1602; 285.1497; 259.1706; 189.0921; 135.0438	2
C4	CBN	9.6	$C_{21}H_{26}O_2$	310.1936	309.1863	309.1860	1.0	309.1860; 279.1391; 171.0816	1
C5	CBD	7.5	$C_{21}H_{30}O_2$	314.2244	313.2171	313.2173	-0.5	313.2173; 311.2018; 245.1553; 191.1078; 179.1067	1
C6	THC	10.7	$C_{21}H_{30}O_2$	314.2243	313.2170	313.2173	-1.0	313.2173; 245.1553; 191.1078; 179.1067	1
C7	CBC	12.0	$C_{21}H_{30}O_2$	314.2242	313.2170	313.2173	-1.1	313.2173; 243.1391; 191.1078; 179.1067	1
C8	CBG	7.3	$C_{21}H_{32}O_2$	316.2401	315.2328	315.2330	-0.6	315.2329; 245.1547; 191.1078; 179.1067	1
C9	CBNVA	7.9	$C_{20}H_{22}O_4$	326.1519	325.1446	325.1445	0.3	325.1443; 281.1548; 251.1068	2
C10	HydroxyCBN	4.9	$C_{21}H_{26}O_3$	326.1885	325.1812	325.1809	0.8	325.1812; 295.1341; 187.0750	2
C11	CBDVA	4.7	$C_{20}H_{26}O_4$	330.1835	329.1762	329.1758	1.1	329.1759; 311.1653; 285.1858; 283.1704; 217.1228; 163.0754; 151.0754	2
C12	THCVA isomer	8.7	$C_{20}H_{26}O_4$	330.1833	329.1761	329.1758	0.7	329.1759; 311.1653; 285.1858; 217.1228; 163.0754; 151.0754	3
C13	THCVA	9.3	$C_{20}H_{26}O_4$	330.1833	329.1760	329.1758	0.6	329.1759; 311.1653; 285.1858; 217.1228; 163.0754; 151.0754	2
C14	CBCVA	10.1	$C_{20}H_{26}O_4$	330.1833	329.1760	329.1758	0.6	329.1759; 311.1653; 285.1858; 215.1072; 163.0754; 151.0754	2
C15	CBE 1	2.9	$C_{21}H_{30}O_3$	330.2198	329.2126	329.2122	1.0	329.2121; 311.2018; 205.1228; 179.1071; 173.0964	2
C16	CBE 2	8.5	$C_{21}H_{30}O_3$	330.2199	329.2126	329.2122	1.2	329.2121; 311.2018; 205.1228; 179.1071; 173.0964	2
C17	CBGVA	5.4	$C_{20}H_{28}O_4$	332.1992	331.1919	331.1915	1.2	331.1916; 313.1812; 287.2018; 217.1228; 163.0754; 151.0754	2
C18	CBDBA	5.7	$C_{21}H_{28}O_4$	344.1989	343.1916	343.1915	0.3	343.1916; 325.1809; 299.2018; 297.1861; 231.1393; 177.0913; 165.0912	2
C19	CBDVMA	9.1	$C_{21}H_{28}O_4$	344.1988	343.1915	343.1915	0.0	343.1915; 299.2015; 297.1860; 231.1388; 165.0912; 150.0676	2
C20	CBCBA	11.6	$C_{21}H_{28}O_4$	344.1987	343.1915	343.1915	-0.1	343.1916; 325.1809; 299.2018; 229.1232; 177.0913; 165.0912	2
C21	THCBA	10.8	$C_{21}H_{28}O_4$	344.1988	343.1915	343.1915	0.0	343.1916; 325.1809; 299.2018; 231.1393; 177.0913; 165.0912	2
C22	CBEVA 3	3.0	$C_{20}H_{26}O_5$	346.1783	345.1711	345.1707	0.9	345.1707; 327.1598; 301.1808; 283.1710; 177.0909; 151.0750	2
C23	CBEVA 1	1.4	$C_{20}H_{26}O_5$	346.1783	345.1711	345.1707	0.9	345.1707; 327.1598; 301.1808; 283.1710; 177.0909; 151.0750	2
C24	CBEVA 2	1.9	$C_{20}H_{26}O_5$	346.1783	345.1711	345.1707	0.9	345.1707; 327.1598; 301.1808; 283.1710; 173.0962; 151.0750	2
C25	CBT 2	3.3	$C_{21}H_{30}O_4$	346.2147	345.2074	345.2071	0.8	345.2046; 327.1964; 309.1860; 285.1863; 191.1078; 179.1067	2
C26	CBT 4	5.3	$C_{21}H_{30}O_4$	346.2147	345.2075	345.2071	0.9	345.2046; 327.1964; 309.1860; 285.1863; 191.1078; 179.1067	2
C27	CBGBA	6.3	$C_{21}H_{30}O_4$	346.2144	345.2072	345.2071	0.1	345.2071; 327.1966; 301.2173; 231.1393; 177.0913; 165.0912	2
C28	CBT 3	3.7	$C_{21}H_{30}O_4$	346.2147	345.2075	345.2071	0.9	345.2046; 327.1964; 309.1860; 285.1863; 191.1078; 179.1067	2
C29	CBT 1	2.3	$C_{21}H_{30}O_4$	346.2148	345.2075	345.2071	1.0	345.2046; 327.1964; 309.1860; 285.1863; 191.1078; 179.1067	2
C30	CBGVMA	10.7	$C_{21}H_{30}O_4$	346.2144	345.2072	345.2071	0.1	345.2071; 327.1607; 301.2176; 217.1227; 163.0754	2
C31	CBNDA	3.8	$C_{22}H_{26}O_4$	354.1832	353.1759	353.1758	0.3	353.1752; 309.1860; 279.1399; 171.0805	2
C32	CBNA	11.0	$C_{22}H_{26}O_4$	354.1832	353.1759	353.1758	0.1	353.1752; 309.1860; 279.1399; 171.0805	2
C33	THCA isomer 2	11.7	$C_{22}H_{30}O_4$	358.2145	357.2072	357.2071	0.2	357.2072; 339.1963; 313.2173; 245.1546; 191.1070; 179.1068	3
C34	THCA isomer 1	11.3	$C_{22}H_{30}O_4$	358.2145	357.2072	357.2071	0.3	357.2072; 339.1963; 313.2173; 245.1546; 191.1070; 179.1068	3
C35	THCA	12.3	$C_{22}H_{30}O_4$	358.2145	357.2072	357.2071	0.2	357.2072; 339.1963; 313.2173; 245.1546; 191.1070; 179.1068	1
C36	CBDA	6.8	$C_{22}H_{30}O_4$	358.2145	357.2072	357.2071	0.2	357.2072; 339.1963; 313.2173; 311.2017; 245.1546; 191.1070; 179.1068	1
C37	CBCA	13.0	$C_{22}H_{30}O_4$	358.2145	357.2072	357.2071	0.2	357.2072; 339.1963; 313.2173; 243.1386; 191.1070; 179.1068	2
C38	CBDA isomer	9.0	$C_{22}H_{30}O_4$	358.2145	357.2072	357.2071	0.3	357.2072; 339.1963; 313.2173; 243.1386; 191.1070; 179.1068	3
C39	CBGA	7.3	$C_{22}H_{32}O_4$	360.2302	359.2229	359.2228	0.3	359.2229; 341.2122; 315.2329; 245.1546; 191.1070; 179.1068	1
C40	CBGA isomer	8.3	$C_{22}H_{32}O_4$	360.2302	359.2229	359.2228	0.3	359.2229; 341.2122; 315.2329; 245.1546; 191.1070; 179.1068	3
C41	CBDMA 1	11.6	$C_{23}H_{32}O_4$	372.2300	371.2228	371.2228	-0.1	371.2229; 327.2339; 303.1603; 259.1704; 193.1227; 178.0991	2
C42	CBDHA	8.0	$C_{23}H_{32}O_4$	372.2301	371.2228	371.2228	0.0	371.2228; 353.2114; 327.2327; 325.2164; 259.1703; 205.1224; 193.1228	2
C43	CBDMA 2	12.0	$C_{23}H_{32}O_4$	372.2299	371.2227	371.2228	-0.4	371.2229; 327.2339; 303.1603; 259.1704; 193.1227; 178.0991	2
C44	CBEA 1	1.9	$C_{22}H_{30}O_5$	374.2097	373.2024	373.2020	1.0	373.2022; 329.2122; 311.2017; 271.1704; 205.1234; 191.1070; 179.1068; 173.0962	2
C45	CBEA 3	3.2	$C_{22}H_{30}O_5$	374.2097	373.2024	373.2020	1.0	373.2022; 329.2122; 311.2017; 271.1704; 205.1234; 191.1070; 179.1068; 173.0962	2
C46	CBEA 5	8.0	$C_{22}H_{30}O_5$	374.2097	373.2024	373.2020	1.0	373.2022; 329.2122; 311.2017; 271.1704; 205.1234; 191.1070; 179.1068; 173.0962	2
C47	CBEA 4	5.4	$C_{22}H_{30}O_5$	374.2097	373.2024	373.2020	1.0	373.2022; 329.2122; 311.2017; 271.1704; 205.1234; 191.1070; 179.1068; 173.0962	2
C48	CBEA 2	2.7	$C_{22}H_{30}O_5$	374.2097	373.2024	373.2020	1.0	373.2023; 355.1916; 329.2122; 311.2018; 191.1069; 179.1070; 173.0963	2
C49	CBGMA	13.1	$C_{23}H_{34}O_4$	374.2461	373.2388	373.2384	0.9	373.2388; 329.2489; 289.1448; 245.1546; 191.1070; 179.1063	2
C50	CBCPA	13.3	$C_{24}H_{34}O_4$	386.2463	385.2390	385.2384	1.5	385.2388; 367.2279; 341.2485; 219.1385; 207.1384	2
C51	CBDPA	9.3	$C_{24}H_{34}O_4$	386.2457	385.2384	385.2384	0.0	385.2388; 367.2279; 341.2485; 339.2330; 273.1863; 207.1384	2
C52	CBGPA	9.6	$C_{24}H_{36}O_4$	388.2614	387.2541	387.2541	0.0	387.2546; 369.2436; 343.2643; 219.1393	2
C53	CBTA	2.6	$C_{22}H_{30}O_6$	390.2048	389.1975	389.1970	1.4	389.1934; 371.1865; 345.2069; 327.1966; 285.1864; 191.1078; 179.1067	2
C54	SesquiCBGA	11.8	$C_{27}H_{40}O_4$	428.2931	427.2858	427.2854	0.9	427.2859; 409.2751; 383.2959; 359.2234; 191.1072	2

Table S4. Flavonoid identification data, comprising compound identity, RT, proposed molecular formula, molecular weight, experimental m/z, calculated m/z, mass error (ppm), major product ions, and confidence level (2a when the position of the conjugation was known, 2b when the position of the conjugation was unknown).

ID	Name	RT (min)	Proposed Formula	Molecular Weight	Experimental m/z	Calculated m/z	Δmass (ppm)	Main product ions	c. l.
F1	(Epi)catechin *O* -hexoside	2.7	$C_{21}H_{24}O_{11}$	452.1325	451.1252	451.1246	1.5	451.1240; 289.0716; 245.0817; 137.0242; 109.0293; 125.0242	2b
F2	(Iso)orientin	10.9	$C_{21}H_{20}O_{11}$	448.1008	447.0935	447.0933	0.5	447.0942; 357.0623; 327.0517; 299.0566; 285.0406; 241.0504; 151.0037; 133.0296; 107.0135	2b
F3	(Iso)orientin isomer 1	15.9	$C_{21}H_{20}O_{11}$	448.1016	447.0943	447.0933	2.3	447.0946; 357.0626; 327.0518; 299.0564; 285.0409; 241.0520; 151.0039; 133.0297; 107.0142	3
F4	(Iso)orientin isomer 2	16.7	$C_{21}H_{20}O_{11}$	448.1019	447.0944	447.0933	2.9	447.0924; 357.0625; 327.0519; 299.0564; 285.0408; 243.0667; 151.0039; 133.0297; 107.0142	3
F5	(Iso)orientin *O* -acetyl-deoxyhexoside	16.2	$C_{29}H_{30}O_{14}$	636.1701	635.1628	635.1618	1.7	635.1626; 593.1547; 575.1403; 473.1096; 357.0620; 327.0513; 309.0406; 285.0403; 241.0508; 133.0293	2b
F6	(Iso)orientin *O* -acetyl-hexoside	15.8	$C_{29}H_{30}O_{15}$	652.1651	651.1578	651.1567	1.7	651.1580; 609.1491; 489.1048; 357.0624; 327.0517; 309.0411; 285.0409; 241.0508; 133.0296	2b
F7	(Iso)orientin *O* -deoxyhexoside 1	11.4	$C_{27}H_{30}O_{15}$	594.1588	593.1515	593.1512	0.5	593.1525; 473.1096; 357.0625; 327.0517; 309.0412; 285.0406; 133.0296; 243.0305; 241.0517	2b
F8	(Iso)orientin *O* -deoxyhexoside 2	14.2	$C_{27}H_{30}O_{15}$	594.1603	593.1530	593.1512	3.0	593.1530; 473.1093; 357.0623; 327.0518; 309.0407; 285.0408; 133.0295; 243.0301; 241.0524	2b
F9	(Iso)orientin *O* -hexoside 1	11.2	$C_{27}H_{30}O_{16}$	610.1536	609.1463	609.1461	0.3	609.1473; 489.1059; 357.0626; 327.0519; 309.0423; 285.0412; 133.0296	2b
F10	(Iso)orientin *O* -hexoside 2	14.3	$C_{27}H_{30}O_{16}$	610.1538	609.1466	609.1461	0.7	609.1478; 489.1051; 357.0625; 327.0519; 309.0410; 285.0406; 133.0296	2b
F11	(Iso)orientin *O* -malonyl-deoxyhexoside 1	13.0	$C_{30}H_{30}O_{18}$	680.1589	679.1517	679.1516	0.1	679.2059; 635.1626; 473.1112; 327.0512; 357.0608; 133.0295	2b
F12	(Iso)orientin *O* -malonyl-deoxyhexoside 2	14.0	$C_{30}H_{30}O_{18}$	680.1599	679.1526	679.1516	1.4	635.1626; 473.1088; 327.0515; 357.0625; 133.0294	2b
F13	(Iso)orientin *O* -pentoside 1	11.4	$C_{26}H_{28}O_{15}$	580.1431	579.1358	579.1355	0.5	579.1367; 519.5410; 459.0939; 357.0626; 327.0517; 309.0412; 285.0408; 133.0296; 151.0036	2b
F14	(Iso)orientin *O* -pentoside 2	13.7	$C_{26}H_{28}O_{15}$	580.1429	579.1357	579.1355	0.2	579.1347; 489.1033; 357.0619; 327.0510; 309.0406; 285.0411; 133.0294; 151.0036	2b
F15	(Iso)vitexin 1	12.1	$C_{21}H_{20}O_{10}$	432.1060	431.0987	431.0984	0.7	431.0990; 341.0667; 311.0567; 283.0618; 269.0461; 117.0347; 107.0142;	2b
F16	(Iso)vitexin 2	18.0	$C_{21}H_{20}O_{10}$	432.1067	431.0994	431.0984	2.3	431.0993; 341.0675; 311.0567; 283.0616; 269.0462; 117.0347	2b
F17	6-Hydroxy luteolin/hypolaetin *O* -glucuronide	12.6	$C_{21}H_{18}O_{13}$	478.0756	477.0684	477.0675	1.9	477.0657; 301.0354; 166.9984; 133.0293; 123.00897	3
F18	6-hydroxy-luteolin/hypolaetin	15.1	$C_{15}H_{10}O_{7}$	302.0437	301.0364	301.0354	3.3	301.0362; 166.9988; 133.0297; 123.0089	3
F19	Acacetin	27.1	$C_{16}H_{12}O_{5}$	284.0688	283.0615	283.0612	1.2	283.0617; 268.0381; 211.0401; 239.0714; 151.0034; 107.0138	2
F20	Acacetin *O* -deoxyhexosyl-hexoside	19.3	$C_{28}H_{32}O_{14}$	592.1442	591.1369	591.1355	2.3	591.1365; 283.0613; 268.0378; 211.0408; 239.0352; 151.0037; 107.0137	2b
F21	Acacetin *O* -glucuronide 1	19.3	$C_{22}H_{20}O_{11}$	460.1019	459.0946	459.0933	2.9	459.0940; 283.0604; 268.0382; 211.0405; 239.0349; 151.0039; 107.0139	2b
F22	Acacetin *O* -glucuronide 2	20.3	$C_{22}H_{20}O_{11}$	460.1009	459.0936	459.0933	0.8	459.0928; 283.0615; 268.0380; 211.0408; 239.0357; 151.0033; 107.0141	2b
F23	Acacetin *O* -hexosyl-glucuronide	17.9	$C_{28}H_{28}O_{16}$	622.1543	621.1470	621.1461	1.5	621.1463; 283.0614; 268.0380; 151.0037	2b
F24	Apigenin	20.9	$C_{15}H_{10}O_{5}$	270.0532	269.0459	269.0455	1.4	269.0456; 227.0355; 225.0555; 151.0035; 117.0345; 107.0137	1
F25	Apigenin isomer 1	15.2	$C_{15}H_{10}O_{5}$	270.0528	269.0455	269.0455	-0.2	269.0462; 227.0355; 225.0557; 151.0036; 117.0347; 107.0139	3
F26	Apigenin isomer 2	18.1	$C_{15}H_{10}O_{5}$	270.0530	269.0457	269.0455	0.5	269.0457; 227.0351; 225.0557; 151.0035; 117.0346; 107.0139	3
F27	Apigenin *O* -deoxyhexosyl-glucuronide	15.3	$C_{27}H_{28}O_{15}$	592.1436	591.1363	591.1355	1.3	591.1359; 269.0458; 227.0354; 225.0562; 151.0037; 117.0346; 107.0138	2b
F28	Apigenin *O* -dihexoside	13.9	$C_{27}H_{30}O_{15}$	594.1599	593.1526	593.1512	2.3	593.1521; 269.0457; 107.0139; 151.0038; 225.0567; 227.0345; 117.0346	2b
F29	Apigenin *O* -glucuronide 1	14.6	$C_{21}H_{18}O_{11}$	446.0859	445.0786	445.0776	2.1	445.0837; 269.0462; 227.0352; 225.0562; 151.0041; 117.0348; 107.0140	2b
F30	Apigenin *O* -glucuronide 2	15.2	$C_{21}H_{18}O_{11}$	446.0851	445.0779	445.0776	0.5	445.0787; 269.0462; 227.0352; 225.0562; 151.0041; 117.0348; 107.0140	2b
F31	Apigenin *O* -glucuronide *O* -hexoside	10.2	$C_{27}H_{28}O_{16}$	608.1378	607.1306	607.1305	0.2	607.1294; 445.0787; 431.0995; 269.0459; 268.0384; 227.1033; 225.0562; 117.0350; 151.0039; 107.0142	2b
F32	Apigenin *O* -pentoside	17.9	$C_{20}H_{18}O_{10}$	402.0960	401.0887	401.0878	2.3	401.0879; 269.0434; 151.0034; 117.0349; 107.0139	2b
F33	Apigenin *O* -pentosyl-hexoside	15.0	$C_{26}H_{28}O_{14}$	564.1490	563.1417	563.1406	2.0	563.1405; 269.0455; 227.0353; 225.0553; 117.0346; 107.0134; 151.0036	2b
F34	Aromadendrin *O* -hexoside 1	6.7	$C_{21}H_{22}O_{11}$	450.1168	449.1096	449.1089	1.4	449.1099; 287.0567; 269.0465; 151.0037; 125.0245; 259.0615	2b
F35	Aromadendrin *O* -hexoside 2	8.2	$C_{21}H_{22}O_{11}$	450.1172	449.1099	449.1089	2.1	449.1099; 287.0567; 269.0460; 259.0616; 125.0245; 151.0038;	2b
F36	Cannflavin A	33.1	$C_{26}H_{28}O_{6}$	436.1877	435.1804	435.1812	-1.8	435.1812; 311.0565; 296.0330; 268.0280	2a
F37	Cannflavin B	30.7	$C_{21}H_{24}O_{6}$	368.1567	367.1194	367.1187	2.0	367.1197; 309.0410; 297.0407; 269.0456	2a
F38	Cannflavin C	32.6	$C_{26}H_{28}O_{6}$	436.1887	435.1814	435.1812	0.5	435.1812; 311.0565; 296.0330; 268.0280	2a
F39	Catechin	7.2	$C_{15}H_{14}O_{6}$	290.0794	289.0721	289.0718	1.1	289.0721; 245.0821; 137.0244; 109.0295; 125.0244	2a
F40	Chrysoeriol	21.7	$C_{16}H_{12}O_{6}$	300.0638	299.0566	299.0561	1.5	299.0565; 284.0330; 257.0413; 255.0304; 151.0037; 107.0139	2b
F41	Chrysoeriol *O* -deoxyhexosyl-glucuronide	15.9	$C_{28}H_{30}O_{16}$	622.1544	621.1471	621.1461	1.6	621.1462; 299.0562; 284.0327; 255.0292; 151.0034; 133.0143; 107.0138	2b
F42	Chrysoeriol *O* -glucuronide	16.0	$C_{22}H_{20}O_{12}$	476.0957	475.0884	475.0882	0.4	475.0897; 299.0568; 284.0333; 255.0296; 151.0041; 107.0138	2b
F43	Chrysoeriol *O* -hexoside	16.3	$C_{22}H_{22}O_{11}$	462.1170	461.1097	461.1089	1.7	461.1110; 299.0562; 284.0327; 257.0410; 255.0298; 151.0032; 107.0136	2b
F44	Chrysoeriol *O* -hexosyl-glucuronide	14.1	$C_{28}H_{30}O_{17}$	638.1493	637.1420	637.1410	1.5	637.1418; 299.0560; 284.0325; 255.0372; 151.0034; 133.0295; 107.0132	2b
F45	Chrysoeriol *O* -malonyl-hexoside	15.7	$C_{25}H_{24}O_{14}$	548.1171	547.1098	547.1093	0.8	503.1199; 341.0668; 299.0523; 298.0483; 284.0330; 255.0309	2b
F46	Chrysoeriol *O* -pentosyl-glucuronide	15.4	$C_{27}H_{28}O_{16}$	608.1389	607.1316	607.1305	1.9	607.1315; 299.0567; 284.0332; 255.0303; 151.0039; 133.0297; 107.0141	2b
F47	Diosmetin	21.9	$C_{16}H_{12}O_{6}$	300.0638	299.0565	299.0561	1.3	299.0563; 284.0328; 257.0408; 255.0309; 151.0036; 107.0138	2b
F48	Diosmetin *O* -deoxyhexosyl-glucuronide	16.3	$C_{28}H_{30}O_{16}$	622.1538	621.1465	621.1461	0.7	621.1456; 299.0563; 284.0328; 255.0303; 151.0037; 133.0143; 107.0138	2b
F49	Diosmetin *O* -glucuronide	16.4	$C_{22}H_{20}O_{12}$	476.0957	475.0885	475.0882	0.5	475.0855; 299.0569; 284.0334; 255.0309; 151.0040; 107.0137	2b
F50	Diosmetin *O* -hexoside	17.1	$C_{22}H_{22}O_{11}$	462.1175	461.1102	461.1089	2.8	461.1110; 299.0562; 284.0327; 257.0410; 255.0298; 151.0032; 107.0136	2b
F51	Diosmetin *O* -hexosyl-glucuronide	14.6	$C_{28}H_{30}O_{17}$	638.1494	637.1421	637.1410	1.6	637.1410; 299.0563; 284.0327; 255.0294; 151.0035; 133.0143; 107.0131	2b
F52	Diosmetin *O* -malonyl-hexoside	15.8	$C_{25}H_{24}O_{15}$	548.1542	547.1469	547.1457	2.1	503.1200; 341.0668; 299.0525; 298.0482; 257.0445	2b
F53	Diosmetin *O* -pentosyl-glucuronide	15.9	$C_{27}H_{28}O_{16}$	608.1388	607.1315	607.1305	1.7	607.1308; 299.0563; 284.0328; 255.0300; 151.0035; 133.0141; 107.0138	2b
F54	Epicatechin	4.0	$C_{15}H_{14}O_{6}$	290.0796	289.0723	289.0718	1.9	289.0717; 245.0819; 137.0244; 109.0293; 125.0242	1
F55	Eriodictyol *O* -dihexoside 1	9.6	$C_{27}H_{32}O_{16}$	612.1698	611.1625	611.1618	1.3	611.1610; 449.1086; 287.0560; 151.0035; 135.0450; 107.0137	2b
F56	Eriodictyol *O* -dihexoside 2	10.6	$C_{27}H_{32}O_{16}$	612.1685	611.1613	611.1618	-0.8	611.1492; 449.1087; 287.0560; 151.0034; 135.0450; 107.0136	2b
F57	Eriodictyol *O* -malonyl-hexoside 1	15.5	$C_{28}H_{28}O_{16}$	536.1179	535.1106	535.1093	2.3	491.1211; 287.0561; 151.0035; 135.0450; 107.0137	2b
F58	Eriodictyol *O* -malonyl-hexoside 2	16.9	$C_{28}H_{28}O_{16}$	536.1180	535.1107	535.1093	2.6	491.1102; 287.0564; 151.0034; 135.0450; 107.0137	2b
F59	Eriodictyol	16.9	$C_{15}H_{12}O_{6}$	288.0643	287.0570	287.0561	3.1	287.0566; 177.0187; 151.0036; 135.0452; 107.0138	1
F60	Eriodictyol *O* -glucuronide	11.9	$C_{21}H_{20}O_{12}$	464.0964	463.0891	463.0882	2.0	463.0889; 287.0563; 151.0036; 135.0451	2b
F61	Eriodictyol *O* -hexoside 1	11.7	$C_{21}H_{22}O_{11}$	450.1171	449.1098	449.1089	1.9	449.1094; 287.0563; 151.0036; 135.0451; 107.0137	2b
F62	Eriodictyol *O* -hexoside 2	13.8	$C_{21}H_{22}O_{11}$	450.1174	449.1101	449.1089	2.6	449.1069; 287.0564; 151.0036; 135.0452; 107.0138; 177.0190	2b
F63	Eriodictyol *O* -hexoside 3	15.0	$C_{21}H_{22}O_{11}$	450.1177	449.1104	449.1089	3.2	449.1074; 287.0562; 151.0034; 135.0450; 107.0136; 177.0192	2b
F64	Hesperetin	21.3	$C_{16}H_{14}O_{6}$	302.0799	301.0726	301.0718	2.7	301.0718; 286.0484; 242.0589; 151.0036; 107.0137; 164.0113; 177.0178	1
F65	Hesperetin *O* -acetyl-hexoside 1	18.0	$C_{24}H_{26}O_{12}$	506.1438	505.1365	505.1352	2.8	301.0796; 286.0486; 151.0036; 107.0138; 164.0115; 177.0191;	2b
F66	Hesperetin *O* -acetyl-hexoside 2	18.6	$C_{24}H_{26}O_{12}$	506.1439	505.1366	505.1352	2.9	505.1362; 301.0723; 286.0488; 242.0589; 177.0200; 151.0037; 107.0138; 164.0117	2b
F67	Hesperetin *O* -glucuronide	16.3	$C_{22}H_{22}O_{12}$	478.1120	477.1047	477.1039	1.8	477.1016; 301.0715; 286.0486; 242.0578; 164.0111; 177.0189; 151.0036; 107.0138	2b
F68	Hesperetin *O* -hexoside 1	15.2	$C_{22}H_{24}O_{11}$	464.1329	463.1256	463.1246	2.2	463.1285; 301.0727; 286.0473; 151.0038; 164.0116; 107.0139	2b
F69	Hesperetin *O* -hexoside 2	16.6	$C_{22}H_{24}O_{11}$	464.1329	463.1256	463.1246	2.2	463.1253; 301.0722; 286.0486; 242.0589; 177.0197; 151.0038; 107.0138; 164.0116	2b
F70	Isorhamnetin	21.9	$C_{16}H_{12}O_{7}$	316.0591	315.0518	315.0510	2.4	315.0516; 300.0278; 271.0254; 255.0302; 151.0035; 300.0278; 107.0139	2a
F71	Isorhamnetin 3-*O* -hexoside 1	15.3	$C_{22}H_{22}O_{12}$	478.1120	477.1047	477.1039	1.8	477.1041; 315.0495; 314.0437; 271.0250; 243.0300; 255.0294; 151.0041; 107.0139; 300.0280	2b
F72	Isorhamnetin 3-*O* -hexoside 2	15.8	$C_{22}H_{22}O_{12}$	478.1122	477.1049	477.1039	2.3	477.1043; 315.0497; 300.0249; 314.0442; 299.0202; 271.0253; 255.0379; 151.0038; 107.0136	2b
F73	Isorhamnetin *O* -glucuronide	14.6	$C_{22}H_{20}O_{13}$	492.0923	491.0850	491.0831	3.9	491.0845; 315.0514; 300.0278; 271.0255; 151.0036; 107.0137	2b
F74	Kaempferol	21.2	$C_{15}H_{10}O_{6}$	286.0481	285.0408	285.0405	1.3	285.0405; 257.0448; 229.0506; 151.0036; 107.0138	1
F75	Kaempferol 3-*O* -acetyl-hexoside	15.5	$C_{23}H_{24}O_{13}$	592.1437	591.1364	591.1355	1.5	489.1044; 447.0939; 285.0400; 284.0327; 257.0459; 151.0033; 107.0135	2a
F76	Kaempferol 3-*O* -deoxyhexosyl hexoside	14.5	$C_{27}H_{30}O_{15}$	594.1602	593.1529	593.1512	2.9	593.1522; 284.0330; 285.0406; 255.0302; 229.0507; 151.0036; 107.0138; 257.0456	2a
F77	Kaempferol 3-*O* -hexoside 1	13.9	$C_{21}H_{20}O_{11}$	448.1012	447.0939	447.0933	1.4	447.0934; 285.0398; 284.0328; 255.0300; 227.0351; 151.0033; 107.0139; 229.0502; 257.0437	2a
F78	Kaempferol 3-*O* -hexoside 2	14.7	$C_{21}H_{20}O_{11}$	448.1013	447.0940	447.0933	1.5	447.0935; 285.0399; 284.0329; 255.0300; 227.0351; 151.0036; 107.0137; 229.0506; 257.0452	2a
F79	Kaempferol 3-*O* -pentoside 1	15.4	$C_{20}H_{18}O_{10}$	418.0911	417.0838	417.0827	2.5	417.0827; 285.0396; 284.0328; 255.02998; 227.0350; 151.0039; 107.0135	2a
F80	Kaempferol 3-*O* -pentoside 2	16.1	$C_{20}H_{18}O_{10}$	418.0909	417.0837	417.0827	2.2	417.0833; 285.0403; 284.0331; 151.0036; 133.0295; 107.0137	2a
F81	Kaempferol *O* -glucuronide *O* -hexoside	12.0	$C_{27}H_{28}O_{17}$	624.1333	623.1260	623.1254	1.0	623.1268; 461.0728; 447.0953; 285.0399; 284.0329; 255.0300; 227.0351; 151.0036; 107.0137; 229.0506; 257.0452	2b
F82	Luteolin	18.5	$C_{15}H_{10}O_{6}$	286.0481	285.0408	285.0405	1.1	285.0408; 243.0312; 241.0503; 151.0037; 133.0295; 107.0140	1
F83	Luteolin *C* -pentoside	13.5	$C_{20}H_{18}O_{10}$	418.0907	417.0835	417.0827	1.8	417.0822; 357.0626; 327.0519; 285.0401; 151.0045; 133.0298;	2b
F84	Luteolin *O* -deoxyhexoside *O* -hexoside	14.1	$C_{27}H_{30}O_{15}$	594.1600	593.1527	593.1512	2.5	593.1517; 285.0403; 243.0302; 241.0505; 151.0037; 107.0139; 133.0294	2b
F85	Luteolin *O* -deoxyhexosyl-hexoside	12.9	$C_{27}H_{30}O_{15}$	594.1229	593.1156	593.1148	1.3	593.1156; 285.0410; 243.0303; 241.0514; 133.0295; 107.0139; 151.0038;	2b
F86	Luteolin *O* -dihexoside 1	11.9	$C_{27}H_{30}O_{16}$	610.1538	609.1465	609.1461	0.6	609.1471; 447.0938; 285.0408; 243.0304; 241.0498;0151.0040; 107.0136	2b
F87	Luteolin *O* -dihexoside 2	12.3	$C_{27}H_{30}O_{16}$	610.1539	609.1466	609.1461	0.8	609.1466; 447.0924; 285.0406; 243.0301; 241.0506; 151.0037; 107.0138	2b
F88	Luteolin *O* -formyl-hexoside	14.6	$C_{22}H_{20}O_{12}$	476.0971	475.0898	475.0882	3.4	475.0876; 285.0408; 243.0301; 241.0510; 151.0037; 107.0138	2b
F89	Luteolin *O* -glucuronide	13.0	$C_{21}H_{18}O_{12}$	462.0801	461.0728	461.0726	0.6	461.0733; 285.0411; 133.0297; 151.0036; 107.0139; 243.0312; 241.0507	2b
F90	Luteolin *O* -glucuronide derivative	21.0	$C_{21}H_{18}O_{12}$	640.1440	639.1367	639.1355	1.8	639.1381; 463.1033; 285.0402; 284.0327; 151.0039	3
F91	Luteolin *O* -hexoside 1	13.1	$C_{21}H_{20}O_{11}$	448.1011	447.0938	447.0933	1.2	447.0940; 285.0407; 243.0309; 241.0509; 151.0038; 133.0297; 107.0138	2b
F92	Luteolin *O* -hexoside 2	15.1	$C_{21}H_{20}O_{11}$	448.1013	447.0940	447.0933	1.7	447.0897; 285.0405; 243.0298; 241.0502; 151.0038; 133.0295	2b
F93	Luteolin *O* -hexoside 3	16.3	$C_{21}H_{20}O_{11}$	448.1012	447.0940	447.0933	1.5	447.0938; 285.0409; 243.0300; 241.0505; 151.0038; 133.0295	2b
F94	Luteolin *O* -malonyl-hexoside	16.5	$C_{24}H_{22}O_{14}$	534.1016	533.0943	533.0937	1.2	489.1047; 285.0407; 151.0038; 133.0296; 107.0139; 243.0295; 241.0516	2b
F95	Malonyl(iso)orientin	13.6	$C_{24}H_{22}O_{14}$	534.1019	533.0946	533.0937	1.8	489.1039; 447.0935; 357.0617; 327.0515; 299.0560; 285.0398; 241.0504; 133.0294; 151.0032	2b
F96	Methyl-aromadendrin	20.5	$C_{16}H_{14}O_{6}$	302.0798	301.0726	301.0718	2.6	301.0721; 286.0485; 177.0194; 151.0036; 125.0245; 107.0138	2a
F97	Methyl-isorhamnetin	23.1	$C_{17}H_{14}O_{7}$	330.0748	329.0675	329.0667	2.5	329.0672; 314.0436; 299.0201; 271.0252; 151.0041; 107.0135	2a
F98	Methyl-luteolin *C* -glucuronide	14.2	$C_{22}H_{20}O_{12}$	476.0969	475.0896	475.0882	3.0	475.0846; 385.0570; 355.0460; 299.0549; 284.0320; 255.0309; 107.0138	2b
F99	Methyl-luteolin *C* -hexoside	13.7	$C_{22}H_{22}O_{11}$	462.1169	461.1096	461.1089	1.5	461.1088; 371.0759; 341.0670; 299.0562; 284.0326; 257.0472; 255.0298; 151.0037; 107.0142	2b
F100	Methyl-luteolin *O* -dihexoside	14.6	$C_{28}H_{32}O_{16}$	624.1703	623.1630	623.1618	2.0	623.1624; 299.0563; 284.0328; 255.0301; 151.0034; 133.0143; 107.0138	2b
F101	Naringenin	19.8	$C_{15}H_{12}O_{5}$	272.0692	271.0619	271.0612	2.6	271.0617; 177.0195; 151.0038; 119.0503; 107.0137	2a
F102	Naringenin *C* -hexoside	10.8	$C_{21}H_{22}O_{10}$	434.1220	433.1147	433.1140	1.6	433.1146; 271.0617; 343.0819; 313.0730; 177.0194; 151.0038; 119.0503; 227.0719	2b
F103	Naringenin *O* -acetyl-hexoside	17.5	$C_{23}H_{24}O_{11}$	476.1329	475.1256	475.1246	2.2	475.0824; 271.0615; 151.0037; 119.0502; 107.0207	2b
F104	Naringenin *O* -dihexoside	9.7	$C_{28}H_{32}O_{15}$	642.1811	641.1738	641.1723	2.3	595.1683; 433.1145; 271.0615; 151.0038; 119.0503; 107.0137	2b
F105	Naringenin *O* -hexoside 1	11.6	$C_{21}H_{22}O_{10}$	434.1220	433.1148	433.1140	1.7	433.1144; 271.0616; 227.0714; 177.0196; 151.0037; 107.0138	2b
F106	Naringenin *O* -hexoside 2	14.1	$C_{21}H_{22}O_{10}$	434.1222	433.1150	433.1140	2.1	433.1143; 271.0614; 227.0717; 177.0194; 151.0036; 107.0138; 119.0502	2b
F107	Naringenin *O* -hexoside 3	16.8	$C_{21}H_{22}O_{10}$	434.1227	433.1154	433.1140	3.2	433.1116; 271.0613; 227.0716; 177.0194; 151.0035; 107.0137; 119.0501	2b
F108	Phloretin *O* -hexoside	15.8	$C_{21}H_{24}O_{10}$	436.1380	435.1307	435.1297	2.4	435.1304; 273.0774; 167.0351; 179.0350; 123.0453	2b
F109	Pinocembrin *O* -glucuronide	20.0	$C_{21}H_{20}O_{11}$	448.1009	447.0995	447.0984	2.6	431.2303; 255.0667; 213.0560; 211.0767; 151.0037; 107.0139	2b
F110	Procyanidin B2	3.7	$C_{30}H_{26}O_{12}$	578.1433	577.1360	576.1287	1.5	577.1375; 451.1049; 425.0892; 407.0779; 289.0724; 245.0461; 137.0244; 125.0245	1
F111	Quercetin	18.4	$C_{15}H_{10}O_{7}$	302.0433	301.0360	301.0354	2.0	301.0357; 273.0405; 245.0454; 178.9985; 151.0036; 121.0295; 107.0139	1
F112	Quercetin 3-*O* -acetyl-hexoside	14.3	$C_{23}H_{24}O_{13}$	506.1070	505.0997	505.0988	1.8	505.0991; 300.0278; 271.0250; 245.0452; 178.09981; 151.0037; 107.0134; 121.0295	2a
F113	Quercetin 3-*O* -rutinoside (rutin)	12.7	$C_{27}H_{30}O_{16}$	610.1539	609.1466	609.1461	0.9	609.1467; 301.0347; 300.0279; 271.0252; 245.0459; 178.9985; 151.0037; 107.0138	1
F114	Quercetin 3-*O* -dihexoside	10.2	$C_{27}H_{30}O_{17}$	626.1488	625.1415	625.1410	0.8	625.1416; 300.0279; 301.0327; 271.0252; 245.0453; 178.9988; 151.0038; 107.0138	2a
F115	Quercetin 3-*O* -glucoside	12.8	$C_{21}H_{20}O_{12}$	464.0965	463.0892	463.0882	2.2	463.0887; 301.0349; 300.0278; 271.0253; 255.0302; 273.0384; 245.0456; 151.0037; 178.9984; 121.0295; 107.0139	1
F116	Quercetin 3-*O* -hexosyl-glucuronide	7.0	$C_{27}H_{28}O_{18}$	640.1272	639.1199	639.1203	-0.6	639.1191; 463.0891; 300.0280; 301.0347; 271.0252; 178.9985; 151.0035; 107.0138	2a
F117	Quercetin 3-*O* -malonyl-hexoside	14.3	$C_{24}H_{22}O_{15}$	550.0973	549.0901	549.0886	2.7	505.0991; 300.0277; 271.0249; 245.0443; 151.0036; 178.9985; 121.0293	2a
F118	Quercetin 3-*O* -pentoside	13.3	$C_{20}H_{18}O_{11}$	434.0855	433.0782	433.0776	1.3	433.0776; 301.0348; 300.0278; 271.0250; 243.0348; 151.0036; 121.0294; 107.0137	2a
F119	Quercetin 3-*O* -trihexoside	9.2	$C_{33}H_{40}O_{22}$	788.2031	787.1959	787.1939	2.5	787.1953; 301.0345; 300.0282; 271.0255; 178.9987; 151.0040; 107.0138; 121.0295	2a
F120	Quercetin *O* -glucuronide 1	12.3	$C_{21}H_{18}O_{13}$	478.0758	477.0685	477.0675	2.2	477.0698; 301.0361; 178.9988; 151.0038; 107.0142	2b
F121	Quercetin *O* -glucuronide 2	12.8	$C_{21}H_{18}O_{13}$	478.0754	477.0681	477.0675	1.4	477.0682; 301.0358; 273.0414; 245.0460; 151.0037; 178.9986; 121.0295; 107.0138	2b
F122	Quercetin *O* -hexoside	15.0	$C_{21}H_{20}O_{12}$	464.0969	463.0896	463.0882	3.1	463.1320; 301.0727; 273.0409; 178.9987; 151.0037; 107.0139; 121.0296	2b
F123	Taxifolin	10.3	$C_{15}H_{12}O_{7}$	304.0590	303.0517	303.0510	2.2	303.0516; 285.0408; 241.0513; 151.0036; 177.0190; 125.0244	1
F124	Taxifolin *O* -glucuronide	3.7	$C_{21}H_{20}O_{13}$	480.0913	479.0840	479.0831	1.8	479.0831; 303.0518; 285.0414; 241.0514; 151.0038; 125.0245; 177.0197; 107.0148	2b
F125	Taxifolin *O* -hexoside 1	4.4	$C_{21}H_{22}O_{12}$	466.1120	465.1047	465.1039	1.8	465.1043; 303.0517; 285.0412; 241.0506; 177.0195; 151.0038; 125.0245	2b
F126	Taxifolin *O* -hexoside 2	8.4	$C_{21}H_{22}O_{12}$	466.1120	465.1047	465.1039	1.9	465.1043; 303.0517; 285.0418; 241.0511; 177.0194; 151.0037; 107.0138; 125.0245	2b
F127	Tricetin *C* -hexoside	9.3	$C_{21}H_{22}O_{12}$	466.0967	463.0894	463.0882	2.6	463.0893; 373.0570; 343.0465; 259.0251; 257.0452; 151.0039; 149.0245; 107.0139	2b
F128	Tricetin *O* -glucuronide	11.0	$C_{21}H_{18}O_{13}$	478.0755	477.0682	477.0675	1.5	477.0681; 301.0358; 259.0251; 257.0452; 151.0039; 149.0245; 107.0139	2b
F129	b-Procyanidin dimer (cat-cat) 1	5.7	$C_{30}H_{26}O_{12}$	578.1431	577.1358	576.1286	1.2	577.1375; 451.1049; 425.0892; 407.0779; 289.0725; 245.0461; 137.0244; 125.0245	2a
F130	b-Procyanidin dimer (cat-cat) 2	6.6	$C_{30}H_{26}O_{12}$	578.1433	577.1360	576.1288	1.5	577.1375; 451.1049; 425.0892; 407.0779; 289.0725; 245.0461; 137.0244; 125.0245

Table S5. Phenolic acid identification data, comprising compound identity, RT, proposed molecular formula, molecular weight, experimental m/z, calculated m/z, mass error (ppm), major product ions, and confidence level (2a when the position of the conjugation was known, 2b when the position of the conjugation was unknown).

ID	Name	RT (min)	Proposed Formula	Molecular Weight	Experimental m/z	Calculated m/z	Δmass (ppm)	Main product ions	c. l.
P1	Gallic acid	0.7	$C_7H_6O_5$	170.0217	169.0144	169.0142	1.1	169.0145; 125.0246	2a
P2	Dihydroxybenzoyl hexoside 1	0.8	$C_{13}H_{16}O_9$	316.0797	315.0724	315.0722	0.9	315.0729; 153.0196; 152.0116; 109.0299; 108.0217	2b
P3	Hydroxybenzoyl hexoside 1	0.9	$C_{13}H_{16}O_8$	300.0849	299.0777	299.0772	1.4	137.0246; 93.0345	2b
P4	Dihydroxybenzoyl hexoside 2	1.2	$C_{13}H_{16}O_9$	316.0797	315.0724	315.0722	0.8	315.0729; 153.0196; 152.0116; 109.0299; 108.0217	2b
P5	Dihydroxybenzoic acid 1	1.4	$C_7H_6O_4$	154.0269	153.0196	153.0193	1.6	153.0196; 109.0299	2a
P6	Dihydroxybenzoyl hexoside 3	1.5	$C_{13}H_{16}O_9$	316.0797	315.0724	315.0722	0.8	315.0729; 153.0196; 109.0299	2b
P7	Caffeoyl gluconide 1	1.7	$C_{15}H_{18}O_{10}$	358.0907	357.0834	357.0827	2.0	357.0835; 195.0511; 179.0352; 177.0412; 159.0299; 135.0453; 129.0195; 99.0053; 75.0083	2b
P8	Dihydroxybenzoyl pentoside 1	2.0	$C_{12}H_{14}O_8$	286.0695	285.0623	285.0616	2.3	285.0624; 153.0194; 109.0296	2b
P9	3-Caffeoyl quinic acid (Neochlorogenic acid)	2.0	$C_{16}H_{18}O_9$	354.0957	353.0884	353.0878	1.7	353.0886; 191.0564; 179.0351; 135.0453	1
P10	Dihydroxybenzoyl hexoside 4	2.2	$C_{13}H_{16}O_9$	316.0798	315.0725	315.0722	1.1	315.0729; 153.0196; 109.0299	2b
P11	Dihydroxybenzoyl pentoside 2	2.3	$C_{12}H_{14}O_8$	286.0695	285.0622	285.0616	2.2	285.0623; 153.0197; 152.0117; 109.0305; 108.0218	2b
P12	Dihydroxybenzoic acid 2	2.5	$C_7H_6O_4$	154.0268	153.0195	153.0193	1.4	153.0195; 109.0297	2a
P13	Hydroxybenzoyl hexoside 2	2.8	$C_{13}H_{16}O_8$	300.0849	299.0777	299.0772	1.4	299.0776; 137.0245; 93.0343	2b
P14	Caffeoyl gluconide 2	2.9	$C_{15}H_{18}O_{10}$	358.0906	357.0833	357.0827	1.7	357.0835; 195.0511; 179.0352; 177.0412; 159.0299; 135.0453; 129.0195; 105.0193; 75.0083	2b
P15	3-Coumaroyl quinic acid A	3.2	$C_{16}H_{18}O_8$	338.1009	337.0936	337.0929	2.2	191.0563; 163.0402; 119.0503	2a
P16	3-Coumaroyl quinic acid B	3.4	$C_{16}H_{18}O_8$	338.1009	337.0936	337.0929	2.2	191.0564; 163.0402; 119.0503	2a
P17	Caffeoyl gluconide 3	3.5	$C_{15}H_{18}O_{10}$	358.0907	357.0834	357.0827	1.8	357.0835; 195.0511; 179.0352; 177.0412; 159.0299; 135.0453; 129.0195; 99.0053; 75.0083	2b
P18	Caffeoyl hexoside	3.8	$C_{15}H_{18}O_9$	342.0954	341.0881	341.0878	0.9	341.0869; 179.0351; 135.0452	2b
P19	Coumaroyl dihexoside 1	3.9	$C_{21}H_{28}O_{13}$	488.1538	487.1466	487.1457	1.7	487.1451; 163.0401; 119.0502	2b
P20	Coumaroyl hexoside 1	4.1	$C_{15}H_{18}O_8$	326.1007	325.0934	325.0929	1.5	163.0401; 119.0502	2b
P21	Feruloyl hexoside 1	4.1	$C_{16}H_{20}O_9$	356.1113	355.1040	355.1035	1.6	193.0508; 178.0274; 149.0609; 134.0375	2b
P22	Coumaroyl hexoside 2	4.3	$C_{15}H_{18}O_8$	326.1007	325.0934	325.0929	1.5	325.0906; 163.0402; 119.0503	2b
P23	Caffeic acid	4.3	$C_9H_8O_4$	180.0424	179.0352	179.0350	0.9	179.0351; 135.0452	1
P24	5-Caffeoyl quinic acid (Chlorogenic acid)	4.4	$C_{16}H_{18}O_9$	354.0957	353.0884	353.0878	1.7	353.0870; 191.0559; 179.0341; 135.0450	2a
P25	Coumaroyl gluconide 1A	4.7	$C_{15}H_{18}O_9$	342.0954	341.0881	341.0878	0.9	341.0880; 195.0513; 177.0405; 163.0402; 147.0301; 129.0195; 119.0503; 105.0193; 75.0083	2b
P26	Feruloyl gluconide 1	4.7	$C_{16}H_{20}O_{10}$	372.1060	371.0987	371.0984	0.9	371.0985; 195.0513; 193.0509; 178.0274; 177.0405; 159.0302; 149.0612; 134.0375; 129.0195; 99.0087; 75.0083	2b
P27	Coumaroyl gluconide 1B	4.9	$C_{15}H_{18}O_9$	342.0954	341.0881	341.0878	1.0	341.0880; 195.0513; 177.0405; 163.0402; 147.0301; 129.0195; 119.0503; 105.0193; 75.0083	2b
P28	3-Feruloyl quinic acid	5.0	$C_{17}H_{20}O_9$	368.1114	367.1041	367.1035	1.8	367.1038; 193.0508; 191.0564; 178.0274; 149.0609; 134.0375	2a
P29	4-Caffeoyl quinic acid (Cryptochlorogenic acid)	5.3	$C_{16}H_{18}O_9$	354.0958	353.0885	353.0878	1.9	353.0870; 191.0559; 179.0341; 173.0456; 135.0450	2a
P30	Coumaroyl pentosylhexoside 1	5.4	$C_{20}H_{26}O_{12}$	458.1433	457.1360	457.1352	1.9	457.1351; 325.0933; 163.0401; 119.0502	2b
P31	Coumaroyl pentosylhexoside 2	5.6	$C_{20}H_{26}O_{12}$	458.1433	457.1360	457.1352	1.8	457.1333; 325.0957; 163.0402; 119.0503	2b
P32	Coumaroyl gluconide 2A	5.7	$C_{15}H_{18}O_9$	342.0954	341.0881	341.0878	0.9	341.0880; 195.0513; 177.0406; 163.0402; 159.0298; 129.0195; 119.0503; 99.0087; 75.0083	2b
P33	Sinapoyl hexoside 1	5.7	$C_{17}H_{22}O_{10}$	386.1218	385.1145	385.1140	1.3	223.0618; 208.0382; 193.0145; 179.0717; 164.0482; 149.0246	2b
P34	Coumaroyl gluconide 2B	5.8	$C_{15}H_{18}O_9$	342.0954	341.0881	341.0878	0.8	341.0880; 195.0513; 177.0406; 163.0402; 159.0298; 129.0195; 119.0503; 99.0087; 75.0083	2b
P35	Caffeoyl pentosylhexoside 1	5.9	$C_{20}H_{26}O_{13}$	474.1378	473.1305	473.1301	0.9	473.1301; 341.0876; 179.0350; 135.0452	2b
P36	4-Coumaroyl quinic acid A	5.9	$C_{16}H_{18}O_8$	338.1010	337.0937	337.0929	2.4	337.0940; 191.0563; 173.0457; 163.0402; 119.0503	2a
P37	Coumaroyl pentosylhexoside 3	5.9	$C_{20}H_{26}O_{12}$	458.1433	457.1360	457.1352	1.9	457.1356; 325.0931; 163.0401; 119.0502	2b
P38	Coumaroyl gluconide 3A	6.3	$C_{15}H_{18}O_9$	342.0954	341.0881	341.0878	0.8	341.0880; 195.0513; 177.0406; 163.0402; 129.0195; 119.0503; 99.0087; 75.0083	2b
P39	Feruloyl hexoside 2	6.3	$C_{16}H_{20}O_9$	356.1112	355.1039	355.1035	1.3	193.0508; 178.0274; 149.0609; 134.0375	2b
P40	Coumaroyl gluconide 3B	6.6	$C_{15}H_{18}O_9$	342.0954	341.0881	341.0878	0.8	341.0880; 195.0513; 177.0406; 163.0402; 129.0195; 119.0503; 99.0087; 75.0083	2b
P41	Feruloyl gluconide 2	6.8	$C_{16}H_{20}O_{10}$	372.1060	371.0987	371.0984	1.0	371.0992; 195.0514; 193.0509; 178.0274; 177.0405; 159.0302; 149.0612; 134.0375; 129.0195; 105.0194; 75.0083	2b
P42	Coumaroyl dihexoside 2	6.8	$C_{21}H_{28}O_{13}$	488.1539	487.1466	487.1457	1.8	487.1461; 307.0828; 163.0401; 119.0502	2b
P43	5-Coumaroyl quinic acid A	6.8	$C_{16}H_{18}O_8$	338.1009	337.0937	337.0929	2.3	337.0940; 191.0563; 173.0457; 163.0401; 119.0503	2a
P44	Coumaric acid A	6.8	$C_9H_8O_3$	164.0475	163.0402	163.0401	0.9	163.0402; 119.0503	2a
P45	Caffeoyl pentosylhexoside 2	7.0	$C_{20}H_{26}O_{13}$	474.1378	473.1305	473.1301	1.0	473.1301; 341.0883; 323.0776; 179.0351; 135.0453	2b
P46	Coumaroyl hexoside 3	7.1	$C_{15}H_{18}O_8$	326.1009	325.0936	325.0929	2.3	325.0930; 163.0399; 119.0501	2b
P47	4-Coumaroyl quinic acid B	7.3	$C_{16}H_{18}O_8$	338.1010	337.0937	337.0929	2.5	337.0940; 191.0563; 173.0457; 163.0402; 119.0503	2a
P48	Caffeoyl gluconolactone 1	7.3	$C_{15}H_{16}O_9$	340.0801	339.0728	339.0722	2.0	179.0352; 177.0409; 135.0454; 129.0196	2b
P49	Coumaroyl hexoside 4	7.4	$C_{15}H_{18}O_8$	326.1008	325.0935	325.0929	1.9	325.0944; 163.0403; 119.0504	2b
P50	Feruloyl pentosylhexoside	7.4	$C_{21}H_{28}O_{13}$	488.1540	487.1467	487.1457	2.1	487.1466; 355.1044; 193.0507; 178.0272; 149.0609; 134.0375	2b
P51	Feruloyl gluconide 3	7.5	$C_{16}H_{20}O_{10}$	372.1060	371.0987	371.0984	0.9	371.0990; 195.0514; 193.0509; 178.0274; 177.0405; 159.0302; 149.0612; 134.0375; 129.0195; 105.0194; 75.0083	2b
P52	Sinapoyl hexoside 2	7.7	$C_{17}H_{22}O_{10}$	386.1217	385.1145	385.1140	1.1	223.0617; 208.0381; 193.0145; 179.0717; 164.0482; 149.0246	2b
P53	Coumaric acid B	7.8	$C_9H_8O_3$	164.0474	163.0402	163.0401	0.5	163.0401; 119.0502	2a
P54	Coumaroyl dihexoside 3	7.8	$C_{21}H_{28}O_{13}$	488.1543	487.1470	487.1457	2.6	487.1455; 307.0828; 163.0401; 119.0502	2b
P55	Caffeoyl shikimic acid 1	7.8	$C_{16}H_{16}O_8$	336.0853	335.0780	335.0772	2.3	335.0777; 179.0350; 173.0451; 135.0452	2b
P56	Caffeoyl gluconolactone 2	8.4	$C_{15}H_{16}O_9$	340.0801	339.0728	339.0722	2.0	339.0723; 179.0352; 177.0409; 135.0454; 129.0196	2b
P57	Coumaroyl gluconolactone 1A	8.4	$C_{15}H_{16}O_8$	324.0852	323.0779	323.0772	2.0	323.0778; 177.0403; 163.0401; 129.0194; 119.0503	2b
P58	5-Feruloyl quinic acid	8.4	$C_{17}H_{20}O_9$	368.1112	367.1039	367.1035	1.3	367.1038; 193.0508; 191.0564; 178.0274; 173.0454; 149.0609; 134.0375	2a
P59	Coumaroyl gluconolactone 1B	8.6	$C_{15}H_{16}O_8$	324.0853	323.0780	323.0772	2.3	323.0778; 177.0403; 163.0401; 129.0194; 119.0503	2b
P60	Coumaroyl pentoside 1	8.6	$C_{14}H_{16}O_7$	296.0898	295.0826	295.0823	0.8	163.0401; 119.0502	2b
P61	4-Feruloyl quinic acid	8.8	$C_{17}H_{20}O_9$	368.1111	367.1038	367.1035	1.0	367.1049; 193.0508; 191.0564; 178.0274; 173.0454; 149.0609; 134.0375	2a
P62	5-Coumaroyl quinic acid B	8.9	$C_{16}H_{18}O_8$	338.1010	337.0938	337.0929	2.6	337.0940; 191.0563; 173.0457; 163.0401; 119.0503	2a
P63	Ferulic acid	8.9	$C_{10}H_{10}O_4$	194.0580	193.0507	193.0506	0.4	193.0510; 178.0274; 149.0610; 134.0376	1
P64	Caffeoyl gluconolactone 3	9.0	$C_{15}H_{16}O_9$	340.0800	339.0727	339.0722	1.7	339.0716; 179.0352; 177.0409; 135.0454; 129.0196	2b
P65	Coumaroyl pentoside 2	9.3	$C_{14}H_{16}O_7$	296.0899	295.0827	295.0823	1.1	163.0401; 119.0502	2b
P66	Coumaroyl gluconolactone 2A	9.4	$C_{15}H_{16}O_8$	324.0851	323.0778	323.0772	1.8	323.0772; 177.0403; 163.0401; 129.0194; 119.0503	2b
P67	Coumaroyl gluconolactone 2B	9.6	$C_{15}H_{16}O_8$	324.0851	323.0778	323.0772	1.8	323.0782; 177.0404; 163.0401; 129.0194; 119.0503	2b
P68	Caffeoyl shikimic acid 2	9.8	$C_{16}H_{16}O_8$	336.0853	335.0780	335.0772	2.2	335.0779; 179.0350; 173.0451; 135.0452	2b
P69	Coumaroyl shikimic acid 1	10.3	$C_{16}H_{16}O_7$	320.0903	319.0830	319.0823	2.2	319.0827; 173.0453; 163.0402; 119.0503	2b
P70	Coumaroyl gluconolactone 3A	10.8	$C_{15}H_{16}O_8$	324.0851	323.0778	323.0772	1.8	323.0780; 177.0406; 163.0401; 129.0194; 119.0503	2b
P71	Coumaroyl gluconolactone 3B	11.1	$C_{15}H_{16}O_8$	324.0851	323.0778	323.0772	1.7	323.0783; 177.0407; 163.0401; 129.0194; 119.0503	2b
P72	Ferulic acid isomer	11.3	$C_{10}H_{10}O_4$	194.0571	193.0498	193.0506	-4.1	193.0510; 178.0274; 149.0610; 134.0376	3
P73	Coumaroyl shikimic acid 2	12.3	$C_{16}H_{16}O_7$	320.0903	319.0830	319.0823	2.1	319.0827; 173.0453; 163.0402; 119.0503	2b
P74	Sinapoyl quinic acid	13.8	$C_{18}H_{22}O_{10}$	398.1223	397.1150	397.1140	2.4	223.0617; 208.0381; 193.0145; 191.0544; 179.0717; 164.0482; 149.0246	2b
P75	3,4-Dicaffeoyl Quinic Acid	14.6	$C_{25}H_{24}O_{12}$	516.1278	515.1205	515.1195	2.0	515.1198; 353.0877; 335.0762; 191.0559; 179.0347; 173.0452; 135.0450	2a
P76	3,5-Dicaffeoyl Quinic Acid	14.9	$C_{25}H_{24}O_{12}$	516.1272	515.1199	515.1195	0.8	353.0876; 191.0558; 179.0347; 135.0450	2a
P77	4,5-Dicaffeoyl Quinic Acid	16.2	$C_{25}H_{24}O_{12}$	516.1270	515.1197	515.1195	0.3	515.1176; 353.0876; 191.0559; 179.0347; 173.0452; 135.0451	2a