

Mul0145	Positive	449.1	287.3	2.45	449.1	Protonated	Cyanidin 3-O-glucoside (Kuromanin)	Anthocyanins	9	9	9	35400000	36500000	31700000	9	9	9	40700000	40600000	40300000
Mul0159	Positive	535.1	287.4	2.81	535.1	Protonated	Cyanidin 3-O-malonylhexoside	Anthocyanins	9	9	9	2590000	2270000	2380000	9	9	9	88300	103000	85500
Mul0150	Positive	595	287.9	2.6	595	Protonated	Cyanidin 3-O-rutinoside (Keracyanin)	Anthocyanins	18600000	2560000	51800	29000000	28000000	28400000	13500000	20700000	18800000	42200000	38400000	41300000
Mul0484	Negative	489.1	285.3	2.82	490.1	[M-H]-	Cyanidin O-acetylhexoside	Anthocyanins	243000	215000	292000	9	9	9	205000	194000	231000	162000	170000	148000
Mul0460	Negative	465.1	285.3	2.41	466.1	[M-H]-	Cyanidin O-syringic acid	Anthocyanins	9	9	9	91500000	1.36E+08	1.38E+08	4150000	6540000	7230000	1.17E+08	1.18E+08	79500000
Mul0165	Positive	303	149.3	2.9	303.24	Protonated	Delphinidin	Anthocyanins	96800	67700	97400	14400	9960	13700	33100	41800	36600	37100	33500	27700
Mul0135	Positive	465.1	303.1	2.3	465.1	Protonated	Delphinidin 3-O-glucoside (Mirtillin)	Anthocyanins	7950000	6120000	9300000	9	9	9	115000	141000	157000	290000	255000	442000
Mul0180	Positive	637.1	303.5	3.16	637.1	Protonated	Delphinidin O-malonyl-malonylhexoside	Anthocyanins	9	9	9	11800	10500	8350	15300	10600	9650	6800	6280	4660
Mul0160	Positive	493	331.7	2.81	493	Protonated	Malvidin 3-O-galactoside	Anthocyanins	9	9	9	60600	157000	52700	26300	37900	44100	339000	136000	196000
Mul0163	Positive	493.2	331.6	2.86	493.2	Protonated	Malvidin 3-O-glucoside (Oenin)	Anthocyanins	9	5030	24800	74900	172000	61900	32600	34100	38500	395000	161000	212000
Mul0148	Positive	433.1	271	2.58	433.1	Protonated	Pelargonidin 3-O-beta-D-glucoside (Callistephin chloride)	Anthocyanins	9	9	9	9	9	9	1910000	2920000	4630000	45100000	47400000	55300000
Mul0146	Positive	595	271.8	2.45	595	Protonated	Pelargonin	Anthocyanins	12600	7790	104000	142000	160000	135000	10600	16800	20900	86300	68600	71700
Mul0173	Positive	463.123	301.4	3	463.123	Protonated	Peonidin O-hexoside	Anthocyanins	9	9	9	8790000	7250000	6860000	225000	232000	269000	3280000	3370000	3160000
Mul0561	Negative	253.06	253.1	4.57	254.058	[M-H]-	7,4'-Dihydroxyflavone	Flavone	4280	8270	11400	6270	2580	2660	17100	12900	16500	8560	6360	9160
Mul0580	Negative	283.069	268	6.77	284.069	[M-H]-	Acacetin	Flavone	7820	5910	17900	9	9	9	9	9	9	2230	3990	2960
Mul0488	Negative	487.1	283.2	2.93	488.1	[M-H]-	Acacetin O-acetyl hexoside	Flavone	92200	49800	100000	9	9	9	9	9	9	26900	21800	19400
Mul0569	Negative	491.1	287.3	5.18	492.1	[M-H]-	Acetyl-eriodictyol O-hexoside	Flavone	9	9	9	9470	11500	12600	12000	17600	13300	6920	9280	11300
Mul0272	Positive	271.053	215.1	5.48	270.0528	[M+H]+	Apigenin	Flavone	112000	140000	382000	27000	35500	34300	122000	97700	337000	142000	151000	147000
Mul0220	Positive	433.106	313.1	3.73	432.1056	[M+H]+	Apigenin 5-O-glucoside	Flavone	28100	23000	102000	784000	909000	692000	46200	70600	159000	440000	484000	497000
Mul0542	Negative	431.1	269.2	4.07	432.1	[M-H]-	Apigenin 7-O-glucoside (Cosmosiin)	Flavone	25100	14800	41000	13800	9	9	61300	50000	66700	44000	33900	40600
Mul0248	Positive	519	271.7	4.36	518	[M+H]+	Apigenin O-malonylhexoside	Flavone	47100	25300	57200	35700	34600	44400	567000	766000	687000	268000	267000	254000
Mul0550	Negative	445.085	269	4.33	446.085	[M-H]-	Baicalein-7-O-glucuronide (Baicalin)	Flavone	9	9	9	18200	24500	15600	9	9	9	5060	5230	5110
Mul0271	Positive	273.07	153.1	5.45	272.069	[M+H]+	Butin	Flavone	426000	426000	136000	1190000	1140000	852000	240000	294000	307000	509000	503000	493000
Mul0291	Positive	255.058	69.7	6.73	254.0579	[M+H]+	Chrysin	Flavone	36200	36500	62400	38100	39400	40300	23500	21800	35000	37000	38300	33700
Mul0259	Positive	417.1	255.7	4.84	416.1	[M+H]+	Chrysin 5-O-glucoside (Toringin)	Flavone	9790	7990	38100	27400	18300	25400	12800	12700	18300	18000	16800	14200
Mul0256	Positive	417.2	255.8	4.67	416.2	[M+H]+	Chrysin O-hexoside	Flavone	9	9	9	14500	14500	11000	8100	7720	24700	9280	10100	10400
Mul0266	Positive	503	255.6	5.24	502	[M+H]+	Chrysin O-malonylhexoside	Flavone	45300	26100	54900	98700	88200	84100	110000	139000	296000	103000	98600	88500
Mul0274	Positive	301.063	286.1	5.56	300.0634	[M+H]+	Chrysoeriol	Flavone	31700	30300	89700	151000	233000	183000	64400	56600	114000	88100	91900	89500
Mul0231	Positive	463.123	313.9	3.96	462.123	[M+H]+	Chrysoeriol 5-O-hexoside	Flavone	9	15000	27800	168000	220000	136000	61500	87000	87600	89000	65900	75800
Mul0241	Positive	463.2	287.7	4.14	462.2	[M+H]+	Chrysoeriol 7-O-hexoside	Flavone	19300	10500	21000	171000	243000	161000	59900	77700	90500	75300	81800	78100
Mul0535	Negative	607.1	299.1	3.93	608.1	[M-H]-	Chrysoeriol 7-O-rutinoside	Flavone	9	9	9	219000	201000	212000	230000	254000	198000	337000	189000	282000
Mul0530	Negative	503.1	341.3	3.88	504.1	[M-H]-	Chrysoeriol O-acetylhexoside	Flavone	263000	384000	406000	22300	9	17400	2860000	2740000	2710000	1430000	859000	1280000
Mul0237	Positive	625.1	331.7	4.03	624.1	[M+H]+	Chrysoeriol O-hexosyl-O-hexoside	Flavone	30900	22900	44100	9	9	9	9	9	9	16500	19000	18100
Mul0198	Positive	509.3	347.9	3.47	508.3	[M+H]+	Limocitrin O-hexoside	Flavone	9	9	9	1030000	1010000	1050000	1010000	855000	985000	714000	665000	614000
Mul0262	Positive	287.1	287.1	4.91	286.1	[M+H]+	Luteolin	Flavone	1630000	1890000	4210000	219000	470000	252000	156000	121000	1060000	1110000	1010000	1030000
Mul0193	Positive	611.1	449.4	3.38	610.1	[M+H]+	Luteolin 3',7-di-O-glucoside	Flavone	597000	492000	1020000	93100	99600	113000	191000	192000	210000	266000	290000	287000
Mul0221	Positive	449	287.1	3.76	448	[M+H]+	Luteolin 7-O-glucoside	Flavone	1020000	1230000	1750000	5190000	9	9	9	9	9	3380000	2580000	2850000
Mul0517	Negative	447.3	285.1	3.7	448.101	[M-H]-	Luteolin 7-O-glucoside (Cynaroside)	Flavone	384000	413000	525000	1250000	985000	646000	317000	333000	362000	631000	588000	578000
Mul0467	Negative	771.1	609.5	2.47	772.1	[M-H]-	Luteolin O-hexosyl-O-hexosyl-O-hexoside	Flavone	3580000	2810000	4040000	6160	9	7310	22400	41800	57200	113000	149000	159000
Mul0294	Positive	403.132	373.1	6.84	402.132	[M+H]+	Nobiletin	Flavone	65800	88500	94900	80900	81400	118000	69700	78200	68600	66300	75900	83800
Mul0267	Positive	477.2	328	5.28	476.2	[M+H]+	O-methylChrysoeriol 7-O-hexoside	Flavone	9	9	9	3400	9	4600	15600	5760	27800	7610	7040	7020
Mul0292	Positive	287.084	287.1	6.73	286.084	[M+H]+	sakuranetin	Flavone	9	9	9	9	9	4780	21600	9	9	4870	4440	4140
Mul0203	Positive	479.118	302.8	3.54	478.118	[M+H]+	Selgin 5-O-hexoside	Flavone	46200	30700	22700	17600	11500	9670	13700	9	9	24100	13900	18600
Mul0243	Positive	565	317.8	4.17	564	[M+H]+	Selgin O-malonylhexoside	Flavone	35400	41500	32700	11900	10400	9490	120000	175000	165000	60900	62700	57300
Mul0223	Positive	509.2	347.6	3.82	508.2	[M+H]+	Syringetin 5-O-hexoside	Flavone	9	9	9	68900	95500	94100	107000	104000	87900	95200	101000	98700
Mul0235	Positive	509.3	283.6	4.02	508.3	[M+H]+	Syringetin 7-O-hexoside	Flavone	9	9	9	20300	19800	24700	9	9	9	6470	5590	8580
Mul0303	Positive	373.121	373.1	7.32	372.121	[M+H]+	Tangeretin	Flavone	60600	96900	81600	86300	75700	122000	69300	71200	67900	71300	78500	87000
Mul0553	Negative	301	149.1	4.38	302.043	[M-H]-	Tricetin	Flavone	89100	83800	78700	19500	30300	20200	15800	18400	22900	37200	38000	43000
Mul0533	Negative	491.1	329.3	3.9	492.1	[M-H]-	Tricin 5-O-hexoside	Flavone	648000	483000	1060000	768000	664000	762000	76600	67700	53400	444000	440000	427000
Mul0536	Negative	637.1	269.3	3.93	638.1	[M-H]-	Tricin 5-O-rutinoside	Flavone	9	9	9	23800	16200	24000	6630	5530	5160	6340	5740	3180
Mul0547	Negative	491.1	431.2	4.14	492.1	[M-H]-	Tricin 7-O-hexoside	Flavone	26200	25500	26400	9	9	9	9	9	9	14300	11100	9120
Mul0189	Positive	655.2	331.7	3.35	654.2	[M+H]+	Tricin 7-O-hexosyl-O-hexoside	Flavone	4560	9	9	51600	52100	44500	31500	33700	39900	42000	29300	29800
Mul0515	Negative	521.1	329.3	3.68	522.1	[M-H]-	Tricin O-saccharic acid	Flavone	2720000	2400000	1720000	2150000	1800000	2570000	613000	617000	496000	1960000	1860000	1850000
Mul0514	Negative	535	329.4	3.68	536	[M-H]-	Tricin O-sinapic acid	Flavone	67800	29900	75700	630000	512000	524000	80900	97600	69100	211000	214000	203000

Mul0556	Negative	287.06	125.1	4.43	288.063	[M-H]-	Aromadedrin (Dihydrokaempferol)	Flavonol	1940000	2220000	480000	608000	944000	935000	746000	486000	751000	1100000	962000	1010000
Mul0191	Positive	321.05	153.1	3.36	320.053	[M+H]+	Dihydromyricetin	Flavonol	9	9	9	83200	42100	75600	96400	72200	39400	35600	34600	30900
Mul0538	Negative	303.058	125.1	3.94	304.058	[M-H]-	Dihydroquercetin (Taxifolin)	Flavonol	9570000	9690000	1680000	3970000	8010000	4790000	5240000	3630000	6870000	6130000	5800000	5750000
Mul0577	Negative	329.1	314.3	5.76	330.1	[M-H]-	Di-O-methylquercetin	Flavonol	1820000	397000	1660000	273000	289000	270000	2150000	1250000	2550000	1230000	1010000	1090000
Mul0211	Positive	289	215.1	3.66	288.063	[M+H]+	Fustin	Flavonol	7610	7560	10200	18100	28900	28500	29200	26400	27300	15800	13000	13500
Mul0565	Negative	675.2	513.2	4.83	676.237	[M-H]-	Icariin (kaempferol 3,7-O-diglucoside 8-prenyl derivative)	Flavonol	29500	40100	27200	9850	9	9	9	9	9	18500	19400	16100
Mul0210	Positive	625.169	317.1	3.64	624.169	[M+H]+	Isorhamnetin 3-O-neohesperidoside	Flavonol	9	9	9	122000	140000	120000	82400	86300	76700	55100	36200	68200
Mul0227	Positive	479.2	317.8	3.86	478.2	[M+H]+	Isorhamnetin 5-O-hexoside	Flavonol	103000	110000	84600	65900	72700	64000	201000	119000	365000	134000	147000	126000
Mul0548	Negative	519.1	315.3	4.22	520.1	[M-H]-	Isorhamnetin O-acetyl-hexoside	Flavonol	26200	23000	21900	2330	9	2160	81600	106000	106000	39000	44400	38400
Mul0244	Positive	479.2	318	4.25	478.2	[M+H]+	Isorhamnetin O-hexoside	Flavonol	98600	105000	94200	59400	57700	59400	196000	146000	380000	141000	117000	117000
Mul0273	Positive	287.048	287	5.52	286.048	[M+H]+	Kaempferol	Flavonol	32900	41400	15200	17400	36500	34900	4660	7840	39300	25900	22400	24800
Mul0213	Positive	579.2	433.1	3.67	578.164	[M+H]+	Kaempferol 3,7-dirhamnoside (Kaempferitrin)	Flavonol	9	9	9	40600	33500	48400	9	17500	21700	13000	13800	13500
Mul0528	Negative	447	284	3.86	448.101	[M-H]-	Kaempferol 3-O-galactoside (Trifolin)	Flavonol	3090000	2350000	3810000	2600000	2120000	2930000	1230000	2180000	1690000	2520000	2420000	2590000
Mul0238	Positive	449.1	287.6	4.03	448.1	[M+H]+	Kaempferol 3-O-glucoside (Astragalin)	Flavonol	343000	196000	356000	242000	232000	195000	85800	138000	108000	208000	193000	187000
Mul0217	Positive	595.159	287	3.7	594.159	[M+H]+	Kaempferol 3-O-robinobioside (Biorobin)	Flavonol	9	9	9	17500000	17500000	15200000	2940000	4480000	2770000	6980000	7000000	6890000
Mul0524	Negative	593.159	285.1	3.77	594.1585	[M-H]-	Kaempferol 3-O-rutinoside (Nicotiflorin)	Flavonol	9	9	9	26800000	23500000	26100000	3010000	4190000	3560000	6980000	6990000	7390000
Mul0503	Negative	739.22	593.3	3.28	740.216	[M-H]-	Kaempferol-3-O-robinoside-7-O-rhamnoside (Robinin)	Flavonol	9	9	9	37200	23500	29200	5820	8600	5220	7790	9270	7970
Mul0264	Positive	333	305.2	4.96	332.053	[M+H]+	Laricitrin	Flavonol	9	6090	9	7490	11000	9710	8030	6100	11000	6450	5460	6220
Mul0225	Positive	479	317.3	3.84	478	[M+H]+	methylquercetin O-hexoside	Flavonol	75600	52600	69100	44200	52900	41200	164000	134000	290000	95400	98800	94100
Mul0567	Negative	301	151.1	4.97	302.04265	[M-H]-	Morin	Flavonol	52300	136000	18800	560000	1470000	722000	47600	50600	202000	519000	273000	378000
Mul0554	Negative	317	179	4.39	318.038	[M-H]-	Myricetin	Flavonol	11900	25500	9530	13500	26700	14600	8850	12300	35500	20400	16800	17600
Mul0506	Negative	479.09	317.3	3.43	480.09	[M-H]-	Myricetin 3-O-galactoside	Flavonol	6220	9	4930	24300	15700	26800	9	3350	3630	8520	9740	7190
Mul0263	Positive	303.043	303	4.92	302.043	[M+H]+	Quercetin	Flavonol	159000	194000	31600	238000	204000	279000	103000	50900	438000	167000	156000	156000
Mul0229	Positive	435.085	303	3.91	434.0849	[M+H]+	Quercetin 3-alpha-L-arabinofuranoside (Avicularin)	Flavonol	7700	8680	9790	300000	322000	255000	26400	42800	55000	95800	132000	91800
Mul0516	Negative	463	301.1	3.68	464.096	[M-H]-	Quercetin 3-O-glucoside (Isotrifoliin)	Flavonol	12500000	10300000	12900000	44800000	43200000	45000000	18400000	25700000	24200000	25900000	26600000	24900000
Mul0201	Positive	611.153	303	3.51	610.153	[M+H]+	Quercetin 3-O-rutinoside (Rutin)	Flavonol	9	9	9	36900000	38300000	31300000	22900000	27300000	22600000	26900000	24900000	26100000
Mul0239	Positive	465	302.9	4.04	464.096	[M+H]+	Quercetin 4'-O-glucoside (Spiraeoside)	Flavonol	17700000	12600000	16600000	29500000	31200000	31600000	21900000	25700000	24100000	26200000	25000000	24900000
Mul0162	Positive	713.1	713.1	2.83	712.1	[M+H]+	Quercetin 5-O-malonylhexosyl-hexoside	Flavonol	403000	420000	453000	9	9	9	1770000	1610000	2090000	331000	385000	407000
Mul0195	Positive	713.1	303.6	3.41	712.1	[M+H]+	Quercetin 7-O-malonylhexosyl-hexoside	Flavonol	169000	134000	162000	9	9	9	229000	199000	151000	105000	163000	112000
Mul0219	Positive	611.2	303.7	3.73	610.2	[M+H]+	Quercetin 7-O-rutinoside	Flavonol	9	9	9	37300000	33000000	34600000	21800000	23800000	22300000	24700000	24300000	23200000
Mul0529	Negative	505.1	301.2	3.87	506.1	[M-H]-	Quercetin O-acetylhexoside	Flavonol	5310000	4110000	6100000	157000	142000	129000	27000000	30400000	20700000	16900000	14600000	15800000
Mul0578	Negative	315	165.1	6.19	316.058	[M-H]-	Rhamnetin (7-O-methyl quercetin)	Flavonol	5100	4890	7350	2190	9	9	3230	3000	3140	4140	3340	3480
Mul0184	Positive	509.1	347.7	3.27	508.1	[M+H]+	Syringetin 3-O-hexoside	Flavonol	9	9	9	181000	174000	222000	243000	195000	250000	127000	128000	98600
Mul0555	Negative	657.1	495.3	4.43	658.1	[M-H]-	Tricin 4'-O-(syringyl alcohol) ether 5-O-hexoside	Flavonolignan	28000	38600	22300	21300	18000	25100	24900	23700	14500	17500	20200	19200
Mul0187	Positive	627.1	447.3	3.33	626.1	[M+H]+	6-C-hexosyl-hesperetin O-hexoside	Flavone C-glycosides	1170000	1090000	1430000	208000	160000	259000	99200	115000	105000	524000	531000	451000
Mul0164	Positive	611.1	329	2.9	610.1	[M+H]+	6-C-hexosyl-luteolin O-hexoside	Flavone C-glycosides	146000	144000	156000	9	9	9	27500	33800	17200	35900	24600	24200
Mul0181	Positive	757.2	757	3.19	756.2	[M+H]+	8-C-hexosyl-apigenin O-hexosyl-O-hexoside	Flavone C-glycosides	9	9	9	35500	25000	42800	15500	12400	11700	14600	12000	17800
Mul0152	Positive	627.1	430	2.65	626.1	[M+H]+	8-C-hexosyl-hesperetin O-hexoside	Flavone C-glycosides	15800000	14200000	19400000	2420000	1580000	2390000	7890000	8160000	10000000	5660000	5450000	5340000
Mul0194	Positive	581.1	449.2	3.38	580.1	[M+H]+	8-C-hexosyl-luteolin O-pentoside	Flavone C-glycosides	20100	20400	9	45800	24700	28100	21300	18300	18800	16900	25700	23700
Mul0228	Positive	433.113	271.7	3.88	432.113	[M+H]+	Apigenin C-glucoside	Flavone C-glycosides	26900	39700	66600	3080	9	2830	9	9	9	14400	15800	11000
Mul0207	Positive	757.3	757.2	3.61	756.3	[M+H]+	C-hexosyl-apigenin O-caffeoylhexoside	Flavone C-glycosides	9	9	9	5800	11900	16000	5490	7790	4690	6360	8790	12200
Mul0206	Positive	757.2	757	3.6	756.2	[M+H]+	C-hexosyl-luteolin O-p-coumaroylhexoside	Flavone C-glycosides	9	9	9	17500	28500	26700	12000	7290	6060	5090	10800	8340
Mul0153	Positive	775.1	774.9	2.68	774.1	[M+H]+	Eriodictiol 6-C-hexoside 8-C-hexoside-O-hexoside	Flavone C-glycosides	9	9	9	28600	25100	27100	19500	30000	21600	11700	18500	15000
Mul0169	Positive	613.1	300.3	2.97	612.1	[M+H]+	Eriodictiol C-hexosyl-O-hexoside	Flavone C-glycosides	863000	773000	1120000	99300	84000	121000	81000	120000	108000	278000	307000	305000

Mul0501	Negative	449.1	329.3	3.21	450.1	[M-H]-	Eriodictyol C-hexoside	Flavone C-glycosides	2700000	1630000	1550000	5260000	7030000	4800000	1510000	1470000	1680000	3080000	3010000	2560000
Mul0208	Positive	433.106	313.1	3.61	432.106	[M+H]+	Isovitexin	Flavone C-glycosides	37600	35800	73200	3140	9	9	9	2150	9	14800	17400	16200
Mul0212	Positive	611.2	299.8	3.67	610.2	[M+H]+	Luteolin 8-C-hexosyl-O-hexoside	Flavone C-glycosides	9	9	9	4870000	4560000	4030000	1230000	1550000	865000	1360000	1570000	1570000
Mul0218	Positive	435.1	339.7	3.73	434.1	[M+H]+	Naringenin C-hexoside	Flavone C-glycosides	21900	13700	19300	9	9	6680	4970	7550	9	4860	6570	11000
Mul0240	Positive	477.1	298	4.06	476.1	[M+H]+	O-methylChrysoeriol 8-C-hexoside	Flavone C-glycosides	55400	44000	44800	9	9	9	9	9	9	16400	14000	12800
Mul0222	Positive	419.1	383.9	3.79	418.1	[M+H]+	O-methylnaringenin C-pentoside	Flavone C-glycosides	9	12100	7410	26400	39500	38300	9	9	9	11900	8000	15100
Mul0186	Positive	275	139.1	3.29	274.084	[M+H]+	Afzelechin (3,5,7,4'-Tetrahydroxyflavan)	Flavanone	16100	14300	2380	29200	47600	56400	35000	18000	54700	24900	24000	34900
Mul0269	Positive	273.1	137.1	5.3	272.069	[M+H]+	Butein	Flavanone	7220000	12100000	8890000	2190000	3000000	2370000	668000	826000	1960000	4610000	4580000	4930000
Mul0260	Positive	289.063	153.1	4.85	288.063	[M+H]+	Eriodictyol	Flavanone	1420000	1730000	453000	12500000	7950000	6440000	710000	1320000	1380000	3460000	3310000	3450000
Mul0250	Positive	537	289.7	4.39	536	[M+H]+	Eriodictyol O-malonylhexoside	Flavanone	14800	9910	12700	481000	661000	335000	25200	76100	65000	117000	120000	104000
Mul0276	Positive	303.079	303.1	5.63	302.079	[M+H]+	Hesperetin	Flavanone	9	9	9	27900	18000	17900	6640	8560	5980	6470	9960	7390
Mul0531	Negative	463.132	301.1	3.88	464.132	[M-H]-	Hesperetin 5-O-glucoside	Flavanone	12600000	11100000	13000000	45000000	42700000	43500000	19600000	27000000	25100000	27100000	26700000	25000000
Mul0546	Negative	609.2	301.3	4.09	610.19	[M-H]-	Hesperetin 7-O-neohesperidoside (Neohesperidin)	Flavanone	9	9	9	7120000	6010000	5540000	747000	596000	628000	1930000	1550000	1430000
Mul0233	Positive	611.19	303	3.99	610.19	[M+H]+	Hesperetin 7-rutinoside (Hesperidin)	Flavanone	9	9	9	17600000	16900000	19800000	3140000	3510000	4390000	7080000	7500000	6800000
Mul0457	Negative	625.2	463.3	2.26	626.2	[M-H]-	Hesperetin O-hexosyl-O-hexoside	Flavanone	9	9	9	5960	9	9	13500	14600	11600	7750	6680	4930
Mul0534	Negative	549.2	387.3	3.93	550.2	[M-H]-	Hesperetin O-malonylhexoside	Flavanone	217000	209000	226000	53200	47600	63400	60800	49100	34700	128000	114000	131000
Mul0575	Negative	301.1	151	5.55	302.27876	[M-H]-	Homoeriodictyol	Flavanone	3270	5360	3780	11700	8070	8960	9	2090	9100	5130	4400	4630
Mul0282	Positive	257	137.1	5.91	256.074	[M+H]+	Isoliquiritigenin	Flavanone	204000	357000	172000	904000	792000	651000	147000	142000	165000	342000	343000	367000
Mul0261	Positive	257	137.1	4.87	256.074	[M+H]+	Liquiritigenin	Flavanone	9	6660	5780	47700	20300	19900	9	5960	9	9750	10500	11300
Mul0573	Negative	271.069	151	5.41	272.0685	[M-H]-	Naringenin	Flavanone	283000	301000	83100	787000	745000	544000	179000	215000	195000	344000	320000	333000
Mul0541	Negative	433.121	122.9	4.05	434.1213	[M-H]-	Naringenin 7-O-glucoside (Prunin)	Flavanone	520000	365000	631000	2230000	2220000	1730000	449000	890000	512000	928000	1060000	975000
Mul0268	Positive	273.07	153.1	5.3	272.069	[M+H]+	Naringenin chalcone	Flavanone	330000	340000	112000	1100000	935000	672000	188000	212000	241000	424000	406000	415000
Mul0253	Positive	521	317.6	4.49	520	[M+H]+	Naringenin O-malonylhexoside	Flavanone	8610	7670	14100	36800	49500	40800	74300	140000	113000	49700	40300	44400
Mul0270	Positive	275.084	107	5.34	274.0841	[M+H]+	Phloretin	Flavanone	11500	6990	9	134000	129000	113000	9	4480	5960	37900	38800	35300
Mul0295	Positive	257.1	153	6.85	256.074	[M+H]+	Pinocembrin (Dihydrochrysin)	Flavanone	11600	5990	9	13600	23400	9420	10200	9540	62300	14800	16400	13300
Mul0324	Positive	355.15	178.9	8.24	354.147	[M+H]+	Xanthohumol	Flavanone	9	9	9	9	9	9	6690	4460	4120	2470	2300	3210
Mul0456	Negative	353.1	191.1	2.21	354.095	[M-H]-	1-O-Caffeoyl quinic acid	Quinate and its derivatives	36200000	42500000	37000000	29700000	31900000	34200000	39900000	37200000	36000000	30300000	38100000	38400000
Mul0197	Positive	369.1	207.5	3.47	368.1	[M+H]+	1-O-Feruloyl quinic acid	Quinate and its derivatives	1000000	1570000	1460000	85100	87000	115000	173000	115000	94600	517000	619000	719000
Mul0167	Positive	369.1	177.5	2.94	368.1	[M+H]+	3-O-Feruloyl quinic acid	Quinate and its derivatives	33700	42500	36500	9	9	9	20300	8890	14200	8320	9540	11200
Mul0508	Negative	337.1	190.9	3.44	338.1	[M-H]-	3-O-p-Coumaroyl quinic acid	Quinate and its derivatives	8510000	7600000	7750000	11300000	10400000	11900000	14300000	11900000	10200000	11100000	10800000	9180000
Mul0463	Negative	499.2	173.2	2.43	500.2	[M-H]-	3-O-p-coumaroyl quinic acid O-hexoside	Quinate and its derivatives	9	9	4260	4990	9	9	29800	24200	15500	10400	4370	10600
Mul0494	Negative	481.1	319.3	3.09	482.1	[M-H]-	3-O-p-coumaroyl shikimic acid O-hexoside	Quinate and its derivatives	9	9	9	44500	74900	36800	9	9	9	11900	15300	11600
Mul0489	Negative	353.1	191.2	2.95	354.1	[M-H]-	4-O-Caffeoyl quinic acid (criptochlorogenic acid)	Quinate and its derivatives	69200	58900	68000	78100	66600	80100	64400	59000	44600	70600	62800	55800
Mul0453	Negative	499.1	163.2	2.18	500.1	[M-H]-	5-O-p-coumaroyl quinic acid O-hexoside	Quinate and its derivatives	15200	7760	11500	22900	17800	22600	31000	22200	18100	15300	14700	21400
Mul0215	Positive	321.1	147.5	3.68	320.1	[M+H]+	5-O-p-Coumaroyl shikimic acid	Quinate and its derivatives	7020	4220	9	9	9	8530	1800000	1980000	974000	304000	288000	259000
Mul0475	Negative	481.1	445.4	2.6	482.1	[M-H]-	5-O-p-coumaroyl shikimic acid O-hexoside	Quinate and its derivatives	9270	7410	11600	143000	162000	173000	15000	17000	15400	50100	46500	43700
Mul0499	Negative	337	275.8	3.18	338	[M-H]-	5-O-p-Coumaroylquinic acid	Quinate and its derivatives	83000	82600	79400	61700	69400	78800	60700	43600	29900	65700	64200	61500
Mul0478	Negative	353.095	191.1	2.69	354.0951	[M-H]-	Chlorogenic acid (3-O-Caffeoylquinic acid)	Quinate and its derivatives	12100000	15200000	14600000	8760000	12200000	7060000	14800000	14500000	20500000	11500000	11400000	11200000
Mul0202	Positive	369.111	163	3.52	368.111	[M+H]+	Chlorogenic acid methyl ester	Quinate and its derivatives	9	9670	4240	29300	8500	28900	11000	6660	4830	10600	9870	10100
Mul0445	Negative	355.1	181.2	1.97	356.1	[M-H]-	Homovanilloyl quinic acid	Quinate and its derivatives	5070000	3320000	4800000	9	9	9	9	9	9	1590000	1440000	1540000
Mul0470	Negative	353	191.1	2.53	354.095	[M-H]-	Neochlorogenic acid (5-O-Caffeoylquinic acid)	Quinate and its derivatives	62500000	56000000	42800000	53800000	55300000	54600000	58400000	57200000	54500000	54700000	51200000	51200000
Mul0507	Negative	709.1	401.3	3.44	710.1	[M-H]-	O-p-Coumaroyl quinic acid O-rutinoside derivative	Quinate and its derivatives	3700	3630	2550	3800	9	9	2510	3250	9	4120	3970	5200
Mul0439	Negative	513.1	191.2	1.86	514.1	[M-H]-	p-Coumaroyl quinic acid O-glucuronic acid	Quinate and its derivatives	87800	34700	78900	9	9	9	22800	12900	5300	21000	29400	22900
Mul0442	Negative	371.1	179.2	1.92	372.1	[M-H]-	Quinacyl syringic acid	Quinate and its derivatives	42900	38400	41800	174000	149000	188000	26800	61800	48700	100000	94500	99800
Mul0413	Negative	191	85	1.22	192.063	[M-H]-	Quinic acid	Quinate and its derivatives	37500000	29200000	25700000	1.04E+08	57700000	82500000	11800000	10600000	11000000	37300000	42400000	43400000
Mul0446	Negative	369	191.1	1.98	370	[M-H]-	Quinic acid O-glucuronic acid	Quinate and its derivatives	54300	94900	68400	189000	136000	137000	81100	106000	77500	178000	80700	152000
Mul0137	Positive	474.2	327.8	2.34	473.2	[M+H]+	10-Formyl-THF	Others	940000	700000	888000	121000	108000	144000	677000	572000	472000	304000	295000	312000
Mul0083	Positive	96.04	80.2	1.21	95.04	[M+H]+	3-Hydroxypyridine	Others	6790	12000	5440	4420	6290	5570	6040	12100	8180	4840	4280	2600
Mul0012	Positive	169.09	134.1	0.66	168.09	[M+H]+	4-(Aminomethyl)-5-(hydroxymethyl)-2-methylpyridin-3-ol	Others	18700	36800	15100	6330	9900	8300	9	9	9	12200	9230	13400
Mul0147	Positive	144.1	142.9	2.55	143.1	[M+H]+	4-Methyl-5-thiazoleethanol	Others	9	5340	5540	7330	4080	6390	4390	4440	9	5940	5170	9150

Mul0009	Positive	140	98.9	0.63	139.027	[M+H] ⁺	4-Nitrophenol	Others	21000000	37200000	21500000	25500000	23200000	29800000	22700000	19200000	19100000	22000000	24200000	27100000
Mul0101	Positive	137	110	1.37	136.039	[M+H] ⁺	Allopurinol	Others	67100	129000	60100	9300	17100	14200	18000	17100	15200	19700	30100	32600
Mul0116	Positive	136.1	119.3	1.83	135.1	[M+H] ⁺	Aminopurine	Others	224000	325000	346000	54100	95700	50500	64100	57100	78200	156000	171000	165000
Mul0166	Positive	491.1	329.7	2.92	490.1	[M+H] ⁺	Anisic acid O-feruloyl hexoside	Others	8370	9300	12700	35500	29800	33900	9	4870	10100	23800	22100	20400
Mul0563	Negative	533.3	371.2	4.71	534.21	[M-H] ⁻	Arctiin	Others	17900	18900	39300	6090	13700	9340	16200	18500	12000	17300	15200	16300
Mul0293	Positive	390.4	284.9	6.74	389.4	[M+H] ⁺	Azoxystrobin acid	Others	131000	326000	201000	269000	259000	346000	155000	158000	182000	192000	240000	225000
Mul0129	Positive	122	105.3	2.19	121	[M+H] ⁺	Benzamide	Others	4500	6270	5690	9360	9820	10300	21900	18400	24000	11900	13200	13200
Mul0308	Positive	387.1	331.8	7.48	386.1	[M+H] ⁺	Cholesterol	Others	106000	138000	129000	152000	139000	196000	129000	124000	132000	110000	127000	151000
Mul0285	Positive	343.1	240.9	6.39	342.1	[M+H] ⁺	Cocamidopropyl betaine	Others	17200	21600	20200	20400	14500	17200	16600	15100	18500	18100	15300	19800
Mul0298	Positive	302.4	284.9	7.15	301.4	[M+H] ⁺	D-erythro-Dihydrosphingosine	Others	8460	8320	11900	137000	34700	107000	9290	9170	8130	18000	22600	18600
Mul0016	Positive	106	88.1	0.68	105.079	[M+H] ⁺	Diethanolamine	Others	44200	44800	54400	18300	40800	20100	26400	29200	40700	33000	37800	26700
Mul0425	Negative	169	122.8	1.25	169.998	[M-H] ⁻	DI-Glyceraldehyde3-phosphate	Others	24600	27500	24200	9	86900	9	41900	51400	48800	52900	56300	56900
Mul0560	Negative	405.13	242.2	4.48	406.13	[M-H] ⁻	E-3,4,5'-Trihydroxy-3'-glucopyranosylstilbene	Others	97100	95800	17300	9	9	9	9	9	9	36700	32100	39200
Mul0003	Positive	142.1	82.9	0.57	141.1	[M+H] ⁺	Histidinol	Others	13100000	24400000	23100000	12100000	14300000	14700000	15400000	12800000	14300000	11700000	14400000	15900000
Mul0099	Positive	138.091	77.2	1.28	137.091	[M+H] ⁺	Hydroxyphenethylamine	Others	38900	54300	32600	33800	26100	62900	12200	10200	10800	12600	16400	12900
Mul0362	Negative	179.157	87	0.74	180.0634	[M-H] ⁻	Inositol	Others	1430000	1090000	1700000	253000	240000	254000	230000	234000	204000	510000	490000	456000
Mul0182	Positive	595.2	367.2	3.19	594.159	[M+H] ⁺	Isovitexin 7-O-glucoside (Saponarin)	Others	9	9	9	19700	11800	35700	30100	39400	26600	21500	14200	11400
Mul0030	Positive	163	103	0.76	162.113	[M+H] ⁺	L-Carnitine	Others	25300	58700	31900	23000	19000	32500	44000	32300	29600	17300	35900	37200
Mul0327	Positive	400.33	341.4	8.31	399.335	[M+H] ⁺	L-Palmitoylcarnitine	Others	9	9	9	22600	10800	23600	11900	8510	4930	6170	8830	7710
Mul0415	Negative	742.1	620.2	1.22	743.075	[M-H] ⁻	NADP	Others	74200	65000	80500	129000	135000	154000	108000	106000	97200	158000	110000	130000
Mul0281	Positive	275.1	258.1	5.9	274.1	[M+H] ⁺	N-Lauryldiethanolamine	Others	55100	46700	53100	96800	86100	101000	82200	92600	74200	65100	73300	72900
Mul0370	Negative	140	78.5	0.76	141.019	[M-H] ⁻	O-Phosphorylethanolamine	Others	21900	12900	20300	19200	29200	14000	33600	35800	37100	34300	24100	21700
Mul0410	Negative	287.06	153.1	1.19	288.059	[M-H] ⁻	Orotidine	Others	66700	50500	39200	9500	13300	10800	9790	8780	5830	16100	16400	16800
Mul0209	Positive	503.2	311.8	3.64	502.2	[M+H] ⁺	Phellodensin F	Others	1360000	1080000	1960000	301000	169000	294000	254000	203000	123000	590000	674000	434000
Mul0141	Positive	122.1	105	2.39	121.089	[M+H] ⁺	Phenethylamine	Others	28400	68400	17900	28000	15000	39400	16900	10800	15300	21900	20800	20100
Mul0348	Positive	149	121.3	9.57	148	[M+H] ⁺	Phthalic anhydride	Others	42500	36100	40000	83700	50400	58900	74800	71900	60900	55500	60600	60200
Mul0496	Negative	385.1	223.2	3.1	386.1	[M-H] ⁻	1-O-beta-D-Glucopyranosyl sinapate	Hydroxycinnamoyl derivatives	116000	94900	260000	73500	60600	78700	584000	486000	447000	236000	210000	234000
Mul0545	Negative	151.047	136.1	4.08	152.0473	[M-H] ⁻	2-Methoxybenzoic acid	Hydroxycinnamoyl derivatives	49200	35500	45100	12800	17300	21000	11300	4840	11000	27200	26000	29000
Mul0204	Positive	167.063	149.1	3.57	166.063	[M+H] ⁺	3-(4-Hydroxyphenyl)propionic acid	Hydroxycinnamoyl derivatives	43400	50700	39100	19500	24600	19900	19300	9	35200	30900	33000	18200
Mul0568	Negative	237.084	103.1	5	238.0841	[M-H] ⁻	3,4,5-Trimethoxycinnamic acid	Hydroxycinnamoyl derivatives	19000	9	9	5330	7620	6490	7170	3540	3870	2860	3510	3210
Mul0574	Negative	207.1	192.1	5.53	208.1	[M-H] ⁻	3,4-Dimethoxycinnamic acid	Hydroxycinnamoyl derivatives	9120	7830	10600	9	9	9	1650	9	9	6040	4460	3760
Mul0540	Negative	193.058	134.1	4.01	194.0579	[M-H] ⁻	3-Hydroxy-4-methoxycinnamic acid	Hydroxycinnamoyl derivatives	324000	351000	220000	111000	184000	175000	193000	210000	172000	228000	224000	229000
Mul0572	Negative	177	145.2	5.36	178	[M-H] ⁻	4-Methoxycinnamic acid	Hydroxycinnamoyl derivatives	264000	261000	132000	2580	4350	3340	20600	12500	13200	95500	92100	91400
Mul0178	Positive	207.1	147.4	3.1	206.1	[M+H] ⁺	6-Hydroxymethylherniarin	Hydroxycinnamoyl derivatives	195000	180000	264000	137000	97500	111000	221000	189000	174000	150000	182000	153000
Mul0310	Positive	317.2	281.3	7.53	316.204	[M+H] ⁺	Cafestol	Hydroxycinnamoyl derivatives	17800	16200	8780	34600	22100	25800	29700	9010	18500	14700	12600	23500
Mul0179	Positive	181.042	135.1	3.14	180.042	[M+H] ⁺	Caffeic acid	Hydroxycinnamoyl derivatives	23800	25300	20700	59600	57600	65900	78000	76700	54300	45000	40800	38600
Mul0492	Negative	341	179.2	3.03	342	[M-H] ⁻	Caffeic acid O-glucoside	Hydroxycinnamoyl derivatives	487000	479000	392000	280000	293000	340000	677000	651000	532000	478000	404000	430000
Mul0279	Positive	165.1	95.5	5.88	164.1	[M+H] ⁺	Caffeic aldehyde	Hydroxycinnamoyl derivatives	9040	4990	7390	7430	9	4150	10500	9680	6010	6620	7770	7140
Mul0452	Negative	311.1	149.2	2.18	312.1	[M-H] ⁻	Caftaric acid	Hydroxycinnamoyl derivatives	9240	6520	10600	51300	43700	51700	9640	9	8800	20200	17900	15400
Mul0571	Negative	147.052	61.8	5.22	148.0524	[M-H] ⁻	Cinnamic acid	Hydroxycinnamoyl derivatives	1240000	1200000	196000	43700	41300	30000	20500	18600	129000	410000	378000	366000
Mul0477	Negative	341	179.1	2.62	342.132	[M-H] ⁻	Coniferin	Hydroxycinnamoyl derivatives	5730000	5180000	5850000	127000	115000	127000	2370000	1990000	1590000	929000	772000	795000
Mul0519	Negative	179.079	146.1	3.71	180.079	[M-H] ⁻	Coniferyl alcohol	Hydroxycinnamoyl derivatives	7970	5440	11000	12800	10500	9730	8230	10000	9	8050	9140	7740
Mul0559	Negative	177.063	177.1	4.46	178.063	[M-H] ⁻	Coniferylaldehyde	Hydroxycinnamoyl derivatives	381000	244000	714000	556000	416000	553000	525000	440000	304000	495000	451000	468000
Mul0230	Positive	195.058	149.1	3.92	194.0579	[M+H] ⁺	Ferulic acid	Hydroxycinnamoyl derivatives	72600	44600	34000	18900	30800	33600	28000	35500	35100	40300	33200	35000
Mul0188	Positive	375.2	137.6	3.34	374.2	[M+H] ⁺	Feruloyl syringic acid	Hydroxycinnamoyl derivatives	14100	26800	28700	21300	18500	19700	9190	9	4780	8210	12400	14700

Mul0185	Positive	183.058	137.1	3.28	182.0579	[M+H] ⁺	Homovanillic acid	Hydroxycinnamoyl derivatives	1120000	793000	1170000	127000	95700	107000	107000	80300	47800	486000	461000	465000
Mul0265	Positive	151.068	105	5.17	150.068	[M+H] ⁺	Hydrocinnamic acid	Hydroxycinnamoyl derivatives	19400	26200	9	9	9	9	9	9	9	9840	9520	10100
Mul0176	Positive	195.1	177.5	3.08	194.1	[M+H] ⁺	Hydroxy-methoxycinnamate	Hydroxycinnamoyl derivatives	84700	71500	55200	13300	8530	12700	27300	15900	20600	42500	44100	41000
Mul0290	Positive	271	137.1	6.67	270.089	[M+H] ⁺	Medicarpin	Hydroxycinnamoyl derivatives	4740	2780	14600	38800	17400	18100	22200	17400	18100	13800	14900	13700
Mul0302	Positive	179	138	7.3	178.099	[M+H] ⁺	Methyleugenol	Hydroxycinnamoyl derivatives	23600	21900	19600	9	9	9	9	9	9	8670	7750	6490
Mul0454	Negative	665.1	323.4	2.19	666.1	[M-H] ⁻	O-Caffeoyl maltotriose	Hydroxycinnamoyl derivatives	30000	18000	24900	9	9	9	9	771	1820	12700	12100	13500
Mul0245	Positive	149.1	131	4.25	148.052	[M+H] ⁺	p-Coumaraldehyde	Hydroxycinnamoyl derivatives	159000	252000	18100	13500	21800	13100	13200	15100	43000	73400	71000	83400
Mul0518	Negative	163.047	119	3.71	164.047	[M-H] ⁻	p-Coumaric acid	Hydroxycinnamoyl derivatives	2640000	3110000	920000	488000	844000	548000	491000	439000	402000	1310000	1240000	1220000
Mul0510	Negative	149	130.1	3.5	150.068	[M-H] ⁻	p-Coumaryl alcohol	Hydroxycinnamoyl derivatives	10100	9	4490	18600	22200	18300	9290	10500	9130	8840	9100	6430
Mul0570	Negative	357.142	136.1	5.18	358.142	[M-H] ⁻	Pinoresinol	Hydroxycinnamoyl derivatives	68400	31600	61700	50200	33800	44200	19100	15700	15600	38700	29400	35500
Mul0562	Negative	227.079	143.1	4.59	228.0786	[M-H] ⁻	Resveratrol	Hydroxycinnamoyl derivatives	82300	100000	52400	614000	330000	440000	22700	24000	33700	168000	161000	151000
Mul0532	Negative	223.069	149.1	3.89	224.069	[M-H] ⁻	Sinapic acid	Hydroxycinnamoyl derivatives	9	9	9	151000	172000	146000	9	26500	30900	49300	43500	48400
Mul0557	Negative	207.1	177.1	4.43	208.074	[M-H] ⁻	Sinapinaldehyde	Hydroxycinnamoyl derivatives	19900	20700	32700	173000	119000	143000	47300	56100	34800	67000	59300	60400
Mul0522	Negative	209	179.1	3.73	210.089	[M-H] ⁻	Sinapyl alcohol	Hydroxycinnamoyl derivatives	9	9	9	148000	126000	144000	9	9	9	34600	41900	28100
Mul0539	Negative	181.1	151.1	3.99	182.1	[M-H] ⁻	Syringaldehyde	Hydroxycinnamoyl derivatives	7780	8390	14900	12300	6250	15100	13800	7550	6210	9090	12600	11000
Mul0482	Negative	371.1	209.2	2.8	372.142	[M-H] ⁻	Syringin	Hydroxycinnamoyl derivatives	154000	146000	161000	183000	183000	173000	55600	127000	141000	155000	150000	132000
Mul0278	Positive	133.058	115	5.83	132.0575	[M+H] ⁺	trans-cinnamaldehyde	Hydroxycinnamoyl derivatives	5670	6480	6790	11400	6950	15100	15200	12800	6630	9840	13400	8560
Mul0502	Negative	167	152.1	3.26	168	[M-H] ⁻	Vanillic acid	Hydroxycinnamoyl derivatives	29900	28400	39700	23100	19400	28000	25900	21300	82600	31900	34800	29900
Mul0214	Positive	219.1	189.5	3.68	218.1	[M+H] ⁺	5-Methoxy-N,N-dimethyltryptamine	Tryptamine derivatives	169000	145000	111000	132000	109000	122000	28200	30400	21600	86400	83800	85800
Mul0156	Positive	161.1	144.2	2.75	160.1	[M+H] ⁺	L-Tryptamine	Tryptamine derivatives	77500	99600	227000	647000	338000	661000	60800	34900	36200	207000	193000	225000
Mul0175	Positive	219	160.1	3.06	218.106	[M+H] ⁺	N-Acetyl-5-hydroxytryptamine	Tryptamine derivatives	28100	21400	33400	37200	35200	33900	54300	69100	71200	53000	39300	31800
Mul0216	Positive	485.1	147.5	3.68	484.1	[M+H] ⁺	N-hexosyl-p-coumaroyl serotonin	Tryptamine derivatives	41500	35600	44500	8180	7890	4900	16700	14900	5740	53600	34100	54100
Mul0103	Positive	177.2	160.5	1.44	176.2	[M+H] ⁺	N-hydroxy tryptamine	Tryptamine derivatives	69300	26100	30200	490000	429000	742000	37300	106000	48700	113000	96300	109000
Mul0110	Positive	177	160.2	1.66	176.095	[M+H] ⁺	serotonin	Tryptamine derivatives	5680000	7960000	6010000	22500000	20700000	24200000	49400000	10400000	9090000	12700000	12900000	13300000
Mul0468	Negative	359.2	179.1	2.5	360.129	[M-H] ⁻	Aminophylline	Alkaloids	17700	17300	18300	9	9	9	35500	32500	20800	16700	16800	11400
Mul0058	Positive	118.1	118.1	0.81	117.079	[M+H] ⁺	Betaine	Alkaloids	165000	435000	165000	84300	90900	57800	74000	62300	122000	97100	87700	137000
Mul0513	Negative	433.121	433	3.6	434.121	[M-H] ⁻	Isohemiphloin	Alkaloids	112000	64500	66400	20900	14900	16300	22400	22000	20500	53300	48900	43500
Mul0074	Positive	86.1	56	1.17	85.1	[M+H] ⁺	Piperidine	Alkaloids	304000	126000	588000	636000	773000	533000	1990000	1850000	1940000	1200000	1120000	1120000
Mul0050	Positive	138	137.9	0.8	137.048	[M+H] ⁺	Trigonelline	Alkaloids	6860000	11200000	8480000	6750000	6430000	7500000	3380000	2900000	2980000	4320000	5090000	5250000
Mul0396	Negative	213.1	78.9	0.97	214.1	[M-H] ⁻	2-Deoxyribose 1-phosphate	Carbohydrates	75800	47400	28300	113000	198000	111000	732000	1010000	983000	428000	450000	435000
Mul0387	Negative	177.14	70.8	0.82	178.048	[M-H] ⁻	D-(+)-Glucono-1,5-lactone	Carbohydrates	167000	155000	69100	83100	97300	108000	28700	37800	36000	54000	71800	53400
Mul0376	Negative	179	70.9	0.77	180.063	[M-H] ⁻	D(+)-Glucose	Carbohydrates	8170000	7860000	3430000	3210000	4750000	3730000	2310000	1900000	2080000	3320000	4100000	3340000
Mul0035	Positive	505.169	127	0.77	504.169	[M+H] ⁺	D(+)-Melezitose	Carbohydrates	64300	49200	106000	54300	90100	74000	97800	73400	75300	60700	74500	66800
Mul0372	Negative	649.1	503.3	0.77	650.1	[M-H] ⁻	D(+)-Melezitose O-rhamnoside	Carbohydrates	37700	34000	63300	30000	64900	21100	120000	108000	161000	104000	72800	105000
Mul0379	Negative	341	58.8	0.78	342.11621	[M-H] ⁻	D-(+)-Sucrose	Carbohydrates	7370000	5320000	7710000	4720000	4270000	5190000	7280000	9030000	7240000	8070000	5070000	5110000
Mul0421	Negative	259	78.8	1.23	260.03	[M-H] ⁻	D-Fructose 6-phosphate	Carbohydrates	242000	241000	263000	469000	688000	462000	1330000	1220000	1220000	845000	762000	746000
Mul0384	Negative	193.141	72.9	0.8	194.043	[M-H] ⁻	D-glucuronic acid	Carbohydrates	217000	224000	129000	446000	769000	430000	988000	1490000	1790000	887000	812000	907000
Mul0398	Negative	259	96.9	0.99	260.03	[M-H] ⁻	D-Glucose 6-phosphate	Carbohydrates	1000000	751000	1120000	5600000	5050000	4910000	5680000	4440000	4300000	4410000	4550000	4030000
Mul0385	Negative	149	58.9	0.81	150.053	[M-H] ⁻	DL-Arabinose	Carbohydrates	1410000	1140000	976000	409000	475000	497000	243000	290000	269000	444000	451000	450000
Mul0424	Negative	289	78.9	1.25	290.04	[M-H] ⁻	D-Sedoheptuose 7-phosphate	Carbohydrates	99600	69900	42400	272000	1080000	9	155000	132000	144000	443000	262000	480000
Mul0402	Negative	289.1	97	1.16	290.1	[M-H] ⁻	Glucarate O-Phosphoric acid	Carbohydrates	235000	170000	79800	9	2850000	9	315000	192000	233000	713000	683000	749000
Mul0004	Positive	197.058	153	0.59	196.0583	[M+H] ⁺	Gluconic acid	Carbohydrates	42700	115000	50400	27400	164000	39000	5120	4260	37800	57000	58500	59900
Mul0007	Positive	180	84.2	0.61	179	[M+H] ⁺	Glucosamine	Carbohydrates	124000	571000	354000	334000	337000	337000	194000	188000	201000	205000	248000	354000
Mul0395	Negative	163	70.8	0.85	164.069	[M-H] ⁻	L-Fucose	Carbohydrates	20000	17000	22600	14200	18600	17400	11000	19800	9	26900	19300	9340
Mul0380	Negative	177.14	74.8	0.78	178.048	[M-H] ⁻	L-Gulonic-γ-lactone	Carbohydrates	42200	54100	9	9	24000	9	9	13500	15600	16300	20400	26000
Mul0373	Negative	665.1	485.3	0.77	666.1	[M-H] ⁻	Maltotetraose	Carbohydrates	15100	24200	18700	14200	18300	19700	19600	13900	20100	19200	15500	15400
Mul0063	Positive	222	138.1	0.83	221.09	[M+H] ⁺	N-Acetyl-D-glucosamine	Carbohydrates	87800	71300	74400	183000	179000	162000	59400	56400	52600	69000	78300	87000

Mul0390	Negative	421.1	241.2	0.83	422.1	[M-H]-	Trehalose 6-phosphate	Carbohydrates	60200	50300	80500	75300	87000	77000	76100	72500	81800	85700	93500	82300
Mul0288	Positive	319.1	301.9	6.63	318.1	[M+H]+	Phytocassane C	Terpenoids	9	9	9	213000	50500	159000	9	9	9	23100	25000	24800
Mul0321	Positive	301.2	133.1	8.15	300.209	[M+H]+	4-Oxoretinol	Vitamins	2880	4560	9	8510	6740	6430	13200	3880	4270	5010	5720	6560
Mul0358	Positive	287.2	173.2	11.2	286.23	[M+H]+	All-trans-13,14-dihydroretinol	Vitamins	4410	1530	3610	5750	5010	6160	3620	4210	3530	4980	4190	4190
Mul0183	Positive	245.09	227.1	3.21	244.088	[M+H]+	Biotin	Vitamins	65200	60200	89100	132000	119000	144000	444000	250000	631000	167000	205000	175000
Mul0130	Positive	220.2	202.7	2.19	219.2	[M+H]+	D-Pantothenic acid	Vitamins	8590000	7200000	11300000	8670000	8520000	9830000	12000000	10800000	9190000	9810000	9660000	9520000
Mul0394	Negative	175	87	0.84	176.12	[M-H]-	L-ascorbate	Vitamins	593000	388000	386000	348000	156000	323000	144000	136000	475000	184000	200000	186000
Mul0104	Positive	123.1	80.3	1.47	122.1	[M+H]+	Niacinamide	Vitamins	50500	82100	61300	53400	33400	32100	63100	59100	45000	43500	45600	48100
Mul0205	Positive	138.05	78	3.58	137.048	[M+H]+	Nicotinic Acid Methyl Ester (Methyl Nicotinate)	Vitamins	9	7370	9	9	9	9	8850	10900	15800	7570	8430	9250
Mul0422	Negative	155	111	1.24	156.017	[M-H]-	Orotic acid	Vitamins	70800	44800	99000	9	9	9	419000	364000	247000	141000	161000	147000
Mul0157	Positive	279.13	149.2	2.78	278.13	[M+H]+	Pantetheine	Vitamins	9	9	9	389000	655000	496000	9	9	9	207000	232000	208000
Mul0091	Positive	170.1	134.1	1.22	169.074	[M+H]+	Pyridoxine	Vitamins	404000	689000	308000	328000	365000	354000	98000	79900	95800	285000	294000	307000
Mul0096	Positive	250	134	1.25	249.04	[M+H]+	Pyridoxine 5'-phosphate	Vitamins	9	3010	9	9	9	9	6290	4420	10100	4760	3110	6500
Mul0102	Positive	494.1	332.8	1.39	493.1	[M+H]+	Pyridoxine di-O-hexoside	Vitamins	10200	13100	11200	4560	5370	9	9	4480	4030	6680	6550	6640
Mul0171	Positive	508.1	152.5	2.98	507.1	[M+H]+	Pyridoxine O-feruloyl hexoside	Vitamins	9	9	9	28500	18300	25800	18700	14400	9510	11700	12600	9450
Mul0076	Positive	332.1	314.7	1.18	331.1	[M+H]+	Pyridoxine O-glucoside	Vitamins	1200000	1150000	1400000	686000	1110000	706000	873000	688000	460000	849000	939000	961000
Mul0495	Negative	375	255.2	3.09	376.138	[M-H]-	Riboflavin	Vitamins	42200	47900	57800	25900	32000	22200	41800	30300	37600	46400	40700	43100
Mul0054	Positive	265.1	140.4	0.81	264.1	[M+H]+	Thiamine	Vitamins	13800	8670	13500	362000	227000	340000	12900	13200	8690	26200	28400	28900
Mul0275	Positive	149.2	107	5.58	148.052	[M+H]+	3,4-Dihydrocoumarin	Coumarins	29400	38200	6470	9	9	9	9	9	8250	11400	13300	13400
Mul0504	Negative	485.1	323.3	3.3	486.1	[M-H]-	4-hydroxycoumarin di-glucoside	Coumarins	9	5010	9	5920	9	6790	6630	7240	6990	5140	6790	3600
Mul0252	Positive	177.047	121	4.46	176.0473	[M+H]+	4-Methylumbelliferone	Coumarins	65000	50700	49200	97900	93100	78300	106000	108000	88700	88300	67500	71700
Mul0154	Positive	353.1	272.8	2.73	352.1	[M+H]+	6,7-dihydroxycoumarin 6-O-quinic acid	Coumarins	62400	142000	109000	60900	39500	49400	166000	128000	128000	86100	67900	95500
Mul0461	Negative	351.1	132.6	2.41	352.1	[M-H]-	6,7-dihydroxycoumarin 7-O-quinic acid	Coumarins	972000	1470000	1280000	300000	280000	264000	1550000	1230000	1060000	962000	621000	787000
Mul0242	Positive	177	121	4.15	176.047	[M+H]+	6-Hydroxy-4-methylcoumarin	Coumarins	39800	13300	22900	52700	52000	50800	61800	77700	62500	45000	37600	37700
Mul0196	Positive	209.2	194.1	3.45	208.037	[M+H]+	6-Methoxy-7,8-DihydroxyCoumarin	Coumarins	146000	129000	195000	9	9	9	251000	256000	193000	124000	137000	107000
Mul0190	Positive	179.03	179	3.35	178.027	[M+H]+	Daphnetin	Coumarins	29200	43000	13700	14700	32200	32500	30000	67900	71700	40800	38000	32100
Mul0498	Negative	177	133.1	3.17	178.027	[M-H]-	Esculetin (6,7-dihydroxycoumarin)	Coumarins	132000	154000	83300	94100	147000	98900	132000	252000	215000	153000	144000	132000
Mul0462	Negative	703.4	351.3	2.42	704.4	[M-H]-	Esculetin O-quinacyl esculetin O-quinic acid	Coumarins	22100	63100	34100	2590	9	4400	67200	50700	45000	23400	13100	13300
Mul0149	Positive	341	179.1	2.58	340.079	[M+H]+	Esculin (6,7-Dihydroxycoumarin-6-glucoside)	Coumarins	1450000	1630000	3300000	409000	318000	450000	5740000	3880000	4290000	917000	954000	924000
Mul0234	Positive	193.1	178.1	4	192.042	[M+H]+	Scopoletin (7-Hydroxy-5-methoxycoumarin)	Coumarins	160000	79100	92900	82000	76400	76300	235000	265000	223000	145000	127000	128000
Mul0047	Positive	256.2	124	0.8	255.2	[M+H]+	Nicotinate ribonucleoside	Nicotinic acid derivatives	8370000	8690000	4880000	4820000	5460000	5100000	3340000	3180000	3260000	4570000	4590000	4620000
Mul0409	Negative	122	77.9	1.19	123	[M-H]-	Nicotinic acid	Nicotinic acid derivatives	224000	170000	82800	9	97200	25100	404000	378000	420000	194000	200000	191000
Mul0118	Positive	286	124.3	1.9	285	[M+H]+	Nicotinic acid-hexoside	Nicotinic acid derivatives	30600	28400	30600	19600	28700	23400	70200	92900	95200	58800	45700	50000
Mul0552	Negative	269	225	4.37	270.053	[M-H]-	2'-Hydroxydaidzein	Isoflavone	4840	5290	4040	9	9	9	10500	13300	14500	7260	6320	7280
Mul0258	Positive	287	217.1	4.79	286.048	[M+H]+	2'-Hydroxygenistein	Isoflavone	1790000	1960000	4500000	248000	516000	280000	163000	123000	1210000	1110000	1140000	1160000
Mul0247	Positive	271	215.2	4.32	270.053	[M+H]+	6-Hydroxydaidzein	Isoflavone	12300	14900	9	6710	8270	5270	3730	5060	3510	6580	10900	4630
Mul0296	Positive	285	270.2	7	284.069	[M+H]+	Biochanin A	Isoflavone	13200	6800	76000	9	9	9	9	9	9	10000	9050	12300
Mul0257	Positive	255.058	199.1	4.75	254.0579	[M+H]+	Daidzein	Isoflavone	9	8930	16800	5730	9	4060	12900	13600	18500	8860	8410	7840
Mul0254	Positive	431.13	267.7	4.54	430.126	[M+H]+	Formononetin 7-O-glucoside (Ononin)	Isoflavone	9	9	9	6760	6010	6660	19000	14600	19600	7920	11000	10100
Mul0226	Positive	433	270.9	3.84	432.106	[M+H]+	Genistein 7-O-Glucoside (Genistin)	Isoflavone	79600	68400	164000	9	9	9	241000	240000	326000	116000	133000	114000
Mul0564	Negative	285.048	257.1	4.83	286.048	[M-H]-	Orobol (5,7,3',4'-tetrahydroxyisoflavone)	Isoflavone	8930	10500	14100	160000	130000	93500	4640	9360	15700	70900	50900	72300
Mul0168	Positive	192.06	114.9	2.95	191.058	[M+H]+	5-Hydroxyindole-3-acetic acid	Indole derivatives	11300	9130	10700	9790	8550	12500	9	9970	3160	12500	9110	9080
Mul0144	Positive	118	58.2	2.41	117	[M+H]+	Indole	Indole derivatives	18800	10200	48900	30500	34900	20500	136000	98800	114000	32200	46800	53500
Mul0249	Positive	146.1	118.1	4.36	145.053	[M+H]+	Indole-3-carboxaldehyde	Indole derivatives	23800	27500	45300	35700	32400	34800	76900	37900	40900	33700	39100	36200
Mul0543	Negative	160.05	116	4.07	161.0477	[M-H]-	Indole-5-carboxylic acid	Indole derivatives	38000	25100	32500	28000	26400	31800	67400	32100	51300	42900	40400	39300
Mul0139	Positive	206.1	147.5	2.39	205.1	[M+H]+	Methoxyindoleacetic acid	Indole derivatives	207000	76000	502000	405000	417000	359000	1920000	1680000	1500000	730000	683000	716000
Mul0428	Negative	147.07	58.8	1.36	148.074	[M-H]-	(Rs)-Mevalonic acid	Organic acids	70800	71600	9	9	215000	9	759000	784000	1120000	428000	401000	338000
Mul0509	Negative	131.08	68.9	3.45	132.079	[M-H]-	(S)-(-)-2-Hydroxyisocaproic acid	Organic acids	57000	40600	34100	23900	32000	44800	53100	49400	124000	62100	48400	39800
Mul0523	Negative	164.04	92	3.76	165.043	[M-H]-	2-(Formylamino)benzoic acid	Organic acids	256000	329000	91800	62600	77500	64000	69400	44300	49400	147000	125000	125000
Mul0486	Negative	153.2	109	2.88	154.027	[M-H]-	2,3-Dihydroxybenzoic acid	Organic acids	215000	169000	146000	569000	552000	518000	217000	229000	245000	838000	499000	489000
Mul0365	Negative	124	79.7	0.75	125.015	[M-H]-	2-Aminoethanesulfonic acid	Organic acids	4920	4860	5950	10100	11700	11400	5290	5600	7770	9800	7410	9870
Mul0480	Negative	175.1	131.3	2.73	176.1	[M-H]-	2-Isopropylmalate	Organic acids	3460000	2280000	3310000	3500000	4190000	3590000	7940000	8450000	8450000	5630000	4970000	4670000
Mul0474	Negative	145.06	101.1	2.58	146.058	[M-H]-	2-Methylglutaric acid	Organic acids	437000	310000	395000	210000	220000	228000	576000	577000	532000	341000	316000	301000
Mul0450	Negative	131.042	86.9	2.15	132.0423	[M-H]-	2-Methylsuccinic acid	Organic acids	2880000	2220000	2270000	2650000	2120000	2550000	3940000	4210000	4310000	3100000	2880000	2920000
Mul0088	Positive	124.03	77.8	1.21	123.032	[M+H]+	2-Picolinic acid	Organic acids	29200	51100	18600	14100	28500	24900	22800	24000	27300	29900	17100	25700

Supplementary Table S2. Differentially accumulated metabolites between CS and HG2.

Index	log2_FC(case_mean/control_mean)	Pvalue	fdr	vip	Ion mode	Q1 (Da)	Q3 (Da)	Rt (min)	Molecular Weight (Da)	Ionization model	Compounds	Class
Mul0541	2.027337085	0.001034	0.006145	1.001731	Negative	433.121	122.9	4.05	434.1213	[M-H]-	Naringenin 7-O-glucoside (Prunin)	Flavanone
Mul0113	-2.398989558	0.001985	0.00935	1.012965	Positive	285.1	153.1	1.74	284.076	[M+H]+	Xanthosine	Nucleotide and its derivatives
Mul0048	-2.355145872	0.016715	0.042795	1.02527	Positive	258.2	125.2	0.8	258.2	Protonated	sn-Glycero-3-phosphocholine	Cholines
Mul0331	-1.06788631	0.006553	0.021504	1.027456	Positive	496.33	478.3	8.49	495.33	[M+H]+	LysoPC 16:0 (2n isomer)	Lipids_Glycerophospholipids
Mul0121	-0.508865055	0.014593	0.038356	1.163724	Positive	166	120.1	1.96	165.079	[M+H]+	L-Phenylalanine	Amino acids
Mul0432	-3.243661038	0.006634	0.02155	1.257786	Negative	282.092	150.1	1.44	283.092	[M-H]-	Guanosine	Nucleotide and its derivatives
Mul0077	10.56313869	0.00054	0.004168	1.406658	Positive	308	162	1.18	307.084	[M+H]+	Glutathione reduced form	Amino acid derivatives
Mul0508	0.49386719	0.00333	0.012761	1.435059	Negative	337.1	190.9	3.44	338.1	[M-H]-	3-O-p-Coumaroyl quinic acid	Quinate and its derivatives
Mul0467	-9.595809975	0.000638	0.004615	1.502298	Negative	771.1	609.5	2.47	772.1	[M-H]-	Luteolin O-hexosyl-O-hexosyl-O-hexoside	Flavone
Mul0501	1.539264337	0.008486	0.02585	1.514385	Negative	449.1	329.3	3.21	450.1	[M-H]-	Eriodictyol C-hexoside	Flavone C-glycosides
Mul0200	-3.266886731	0.002752	0.011118	1.547779	Positive	558.282	264.8	3.5	557.282	[M+H]+	N', N''-disinapoylspermidine	Phenolamides
Mul0511	-3.658848904	0.009483	0.028137	1.575244	Negative	121.04	91.9	3.58	122.037	[M-H]-	4-Hydroxybenzaldehyde	Benzoic acid derivatives
Mul0398	2.438216825	5.79E-05	0.001186	1.670083	Negative	259	96.9	0.99	260.03	[M-H]-	D-Glucose 6-phosphate	Carbohydrates
Mul0445	-18.89805373	0.001273	0.007201	1.681785	Negative	355.1	181.2	1.97	356.1	[M-H]-	Homovanilloyl quinic acid	Quinate and its derivatives
Mul0212	18.92728757	5.25E-05	0.001114	1.720114	Positive	611.2	299.8	3.67	610.2	[M+H]+	Luteolin 8-C-hexosyl-O-hexoside	Flavone C-glycosides
Mul0418	-19.00957108	3.98E-05	0.000946	1.771973	Negative	133	70.8	1.23	134.022	[M-H]-	L(-)-Malic acid	Organic acids
Mul0529	-5.180373951	0.000963	0.005779	1.803986	Negative	505.1	301.2	3.87	506.1	[M-H]-	Quercetin O-acetylhexoside	Flavonol
Mul0039	-1.227209438	0.006393	0.021097	1.818014	Positive	104.1	60.2	0.78	103.1	[M+H]+	Choline	Cholines
Mul0427	-2.282147941	0.02086	0.050782	1.855011	Negative	117.03	99.9	1.31	118.027	[M-H]-	Succinic acid	Organic acids
Mul0456	-0.272291303	0.048768	0.097209	1.894683	Negative	353.1	191.1	2.21	354.095	[M-H]-	1-O-Caffeoyl quinic acid	Quinate and its derivatives
Mul0477	-5.505257523	1.21E-05	0.000513	1.901403	Negative	341	179.1	2.62	342.132	[M-H]-	Coniferin	Hydroxycinnamoyl derivatives
Mul0546	19.39933109	0.000186	0.002245	2.020545	Negative	609.2	301.3	4.09	610.19	[M-H]-	Hesperetin 7-O-neohesperidoside (Neohesperidin)	Flavanone
Mul0269	-1.899748526	0.009051	0.027154	2.05525	Positive	273.1	137.1	5.3	272.069	[M+H]+	Butein	Flavanone
Mul0356	1.287980763	0.034145	0.073221	2.099873	Positive	355.1	337.9	10.36	354.1	[M+H]+	MAG (18:2)	Lipids_Glycerolipids
Mul0120	0.876953311	0.000924	0.0056	2.135517	Positive	167.1	121	1.95	166.1	[M+H]+	6-Methylmercaptapurine	Nucleotide and its derivatives
Mul0260	2.899799198	0.01403	0.037039	2.15444	Positive	289.063	153.1	4.85	288.063	[M+H]+	Eriodictyol	Flavanone
Mul0588	1.098883608	0.018616	0.045882	2.223973	Negative	452	255.3	8.57	453	[M-H]-	LysoPE 16:0	Lipids_Glycerophospholipids
Mul0287	5.69939239	0.040924	0.084996	2.228317	Positive	318.3	300.9	6.63	317.3	[M+H]+	4-Hydroxysphinganine	Lipids_Fatty acids
Mul0173	19.69395676	0.000205	0.002245	2.237187	Positive	463.123	301.4	3	463.123	Protonated	Peonidin O-hexoside	Anthocyanins
Mul0135	-19.7232669	0.001073	0.006308	2.243324	Positive	465.1	303.1	2.3	465.1	Protonated	Delphinidin 3-O-glucoside (Mirtillin)	Anthocyanins
Mul0094	-1.812711101	0.012839	0.034809	2.289364	Positive	130	83.9	1.24	129.043	[M+H]+	5-oxoproline	Amino acid derivatives
Mul0097	0.762549204	0.041176	0.085222	2.820262	Positive	132.1	86	1.27	131.0946	[M+H]+	L-Leucine	Amino acids
Mul0434	1.500853831	0.003003	0.011811	2.895807	Negative	117.02	100	1.55	118.0266	[M-H]-	Methylmalonic acid	Organic acids
Mul0140	20.50903097	0.005223	0.018313	2.89635	Positive	611.2	611.1	2.39	610.2	[M+H]+	Gallocatechin-gallocatechin	Catechin derivatives
Mul0084	-4.043480702	0.000267	0.002597	3.037874	Positive	136.1	136.1	1.21	135.0545	[M+H]+	Adenine	Nucleotide and its derivatives
Mul0152	-2.950623206	0.000783	0.005129	3.050458	Positive	627.1	430	2.65	626.1	[M+H]+	8-C-hexosyl-hesperetin O-hexoside	Flavone C-glycosides
Mul0239	0.976742725	0.000837	0.005254	3.133984	Positive	465	302.9	4.04	464.096	[M+H]+	Quercetin 4'-O-glucoside (Spiraeoside)	Flavonol
Mul0444	-4.862336215	0.002409	0.010282	3.16846	Negative	299.1	137.2	1.96	300.1	[M-H]-	Salicylic acid O-glucoside	Phytohormones
Mul0110	1.778219279	0.00021	0.002245	3.231089	Positive	177	160.2	1.66	176.095	[M+H]+	serotonin	Tryptamine derivatives
Mul0315	-3.829398985	0.002019	0.009367	3.303221	Positive	494.3	184.6	7.71	493.3	[M+H]+	LysoPC 16:1 (2n isomer)	Lipids_Glycerophospholipids
Mul0217	20.82629653	2.61E-05	0.000815	3.324847	Positive	595.159	287	3.7	594.159	[M+H]+	Kaempferol 3-O-robinobioside (Biorobin)	Flavonol
Mul0043	-3.07098746	0.000203	0.002245	3.337993	Positive	116.1	70	0.79	115.0633	[M+H]+	L-Proline	Amino acids
Mul0233	20.93956136	3.21E-05	0.000929	3.458859	Positive	611.19	303	3.99	610.19	[M+H]+	Hesperetin 7-rutinoside (Hesperidin)	Flavanone
Mul0524	21.4321818	1.43E-05	0.000532	4.10533	Negative	593.159	285.1	3.77	594.1585	[M-H]-	Kaempferol 3-O-rutinoside (Nicotiflorin)	Flavonol
Mul0150	5.299932504	1.71E-06	0.00023	4.29001	Positive	595	287.9	2.6	595	Protonated	Cyanidin 3-O-rutinoside (Keracyanin)	Anthocyanins
Mul0531	1.837915752	3.77E-06	0.00032	4.568975	Negative	463.132	301.1	3.88	464.132	[M-H]-	Hesperetin 5-O-glucoside	Flavanone
Mul0516	1.897430266	5.15E-06	0.000383	4.635996	Negative	463	301.1	3.68	464.096	[M-H]-	Quercetin 3-O-glucoside (Isotrifoliin)	Flavonol
Mul0544	-6.951442914	0.000477	0.003778	4.702795	Negative	137	92.8	4.07	138.032	[M-H]-	Quercetin 3-O-glucoside (Isotrifoliin)	Phytohormones
Mul0145	21.87156126	1.85E-05	0.000611	4.778036	Positive	449.1	287.3	2.45	449.1	Protonated	Cyanidin 3-O-glucoside (Kuromanin)	Anthocyanins
Mul0219	21.88955193	9.86E-06	0.000513	4.811314	Positive	611.2	303.7	3.73	610.2	[M+H]+	Quercetin 7-O-rutinoside	Flavonol
Mul0201	21.91139069	7.71E-05	0.001275	4.835073	Positive	611.153	303	3.51	610.153	[M+H]+	Quercetin 3-O-rutinoside (Rutin)	Flavonol
Mul0413	1.402098444	0.02159	0.051711	5.435027	Negative	191	85	1.22	192.063	[M-H]-	Quinic acid	Quinate and its derivatives
Mul0460	23.69040866	0.001307	0.007255	8.860092	Negative	465.1	285.3	2.41	466.1	[M-H]-	Cyanidin O-syringic acid	Anthocyanins

Supplementary Table S3. Differentially accumulated metabolites between CS and BYW.

Index	log2_FC(case_mean/control_mean)	Pvalue	fdr	vip	Ion mode	Q1 (Da)	Q3 (Da)	Rt (min)	Molecular Weight (Da)	Ionization model	Compounds	Class
Mul0097	1.124666	0.00649	0.023086	4.318728	Positive	132.1	86	1.27	131.0946	[M+H] ⁺	L-Leucine	Amino acids
Mul0092	1.117448	0.007765	0.02539	4.263655	Positive	132	85.9	1.23	131.0946	[M+H] ⁺	L-Isoleucine	Amino acids
Mul0056	2.158148	0.000681	0.00586	3.360313	Positive	118.1	71.8	0.81	117.079	[M+H] ⁺	L-Valine	Amino acids
Mul0064	2.08429	0.000845	0.006692	3.209017	Positive	118	88	0.85	117.079	[M+H] ⁺	DL-Norvaline	Amino acids
Mul0374	2.668951	0.000403	0.004583	1.989719	Negative	132	99.9	0.77	133.0375	[M-H] ⁻	L-Aspartic acid	Amino acids
Mul0367	0.915354	0.041563	0.079897	1.96791	Negative	131.054	71.8	0.75	132.054	[M-H] ⁻	L-Asparagine	Amino acids
Mul0078	3.112818	0.00051	0.005029	1.950255	Positive	150	72.8	1.18	149.051	[M+H] ⁺	L-Methionine	Amino acids
Mul0375	-0.94945	0.042971	0.081138	1.91341	Negative	146.1	102.1	0.77	147.0532	[M-H] ⁻	L-Glutamic acid	Amino acids
Mul0121	-0.87122	0.003195	0.015183	1.644755	Positive	166	120.1	1.96	165.079	[M+H] ⁺	L-Phenylalanine	Amino acids
Mul0412	4.78118	4.59E-06	0.000545	1.027776	Negative	180.1	163	1.21	181.074	[M-H] ⁻	L-(-)-Tyrosine	Amino acids
Mul0094	1.006717	0.006662	0.023361	3.049811	Positive	130	83.9	1.24	129.043	[M+H] ⁺	5-oxoproline	Amino acid derivatives
Mul0443	-2.09068	0.022487	0.050981	2.817771	Negative	315.1	152.1	1.93	316.1	[M-H] ⁻	2,5-dihydroxy benzoic acid O-hexside	Benzoic acid derivatives
Mul0511	-3.64115	0.009503	0.029145	1.75573	Negative	121.04	91.9	3.58	122.037	[M-H] ⁻	4-Hydroxybenzaldehyde	Benzoic acid derivatives
Mul0048	-2.64714	0.01332	0.036128	1.175339	Positive	258.2	125.2	0.8	258.2	Protonated	sn-Glycero-3-phosphocholine	Cholines
Mul0471	1.691029	0.00176	0.011487	1.115058	Negative	315.1	153.2	2.55	316.1	[M-H] ⁻	Protocatechuic acid O-glucoside	Catechin derivatives
Mul0200	-4.05889	0.00224	0.013176	1.764355	Positive	558.282	264.8	3.5	557.282	[M+H] ⁺	N', N''-disinapoylspermidine	Phenolamides
Mul0001	-0.47896	0.047683	0.086882	1.519562	Positive	203	112	0.54	202	[M+H] ⁺	Spermine	Phenolamides
Mul0120	1.597067	3.10E-05	0.002292	3.735124	Positive	167.1	121	1.95	166.1	[M+H] ⁺	6-Methylmercaptapurine	Nucleotide and its derivatives
Mul0084	-1.7892	0.000868	0.006781	2.904392	Positive	136.1	136.1	1.21	135.0545	[M+H] ⁺	Adenine	Nucleotide and its derivatives
Mul0117	-0.21882	0.003038	0.014654	1.638581	Positive	268.097	136.1	1.89	267.097	[M+H] ⁺	Adenosine	Nucleotide and its derivatives
Mul0051	-2.76812	0.041785	0.080066	1.616941	Positive	244.086	111.4	0.8	243.086	[M+H] ⁺	Cytidine	Nucleotide and its derivatives
Mul0404	2.915608	0.002827	0.014412	1.365623	Negative	565.1	323.3	1.18	566.1	[M-H] ⁻	Uridine 5'-diphospho-D-glucose	Nucleotide and its derivatives
Mul0432	-1.68863	0.015947	0.040483	1.199821	Negative	282.092	150.1	1.44	283.092	[M-H] ⁻	Guanosine	Nucleotide and its derivatives
Mul0155	1.919365	0.010725	0.031437	1.153718	Positive	298	135.1	2.73	297.09	[M+H] ⁺	5'-Deoxy-5'-(methylthio)adenosine	Nucleotide and its derivatives
Mul0113	-1.60372	0.003963	0.017438	1.015391	Positive	285.1	153.1	1.74	284.076	[M+H] ⁺	Xanthosine	Nucleotide and its derivatives
Mul0150	4.611689	0.001607	0.010723	3.691561	Positive	595	287.9	2.6	595	Protonated	Cyanidin 3-O-rutinoside (Keracyanin)	Anthocyanins
Mul0135	-5.82237	0.001149	0.00822	2.472055	Positive	465.1	303.1	2.3	465.1	Protonated	Delphinidin 3-O-glucoside (Mirtillin)	Anthocyanins
Mul0460	19.34018	0.003059	0.014654	2.170691	Negative	465.1	285.3	2.41	466.1	[M-H] ⁻	Cyanidin O-syringic acid	Anthocyanins
Mul0148	18.41852	0.016506	0.04093	1.515909	Positive	433.1	271	2.58	433.1	Protonated	Pelargonidin 3-O-beta-D-glucoside (Callistephin chloride)	Anthocyanins
Mul0467	-6.42483	0.000665	0.005812	1.661539	Negative	771.1	609.5	2.47	772.1	[M-H] ⁻	Luteolin O-hexosyl-O-hexosyl-O-hexoside	Flavone
Mul0530	2.980343	2.90E-06	0.000441	1.403585	Negative	503.1	341.3	3.88	504.1	[M-H] ⁻	Chrysoeriol O-acetylhexoside	Flavone
Mul0515	-1.98656	0.004594	0.01903	1.142585	Negative	521.1	329.3	3.68	522.1	[M-H] ⁻	Tricin O-saccharic acid	Flavone
Mul0221	-17.1767	0.003556	0.015933	1.020276	Positive	449	287.1	3.76	448	[M+H] ⁺	Luteolin 7-O-glucoside	Flavone
Mul0201	21.36255	8.98E-05	0.002424	4.459434	Positive	611.153	303	3.51	610.153	[M+H] ⁺	Quercetin 3-O-rutinoside (Rutin)	Flavonol
Mul0219	21.26202	2.97E-06	0.000441	4.306888	Positive	611.2	303.7	3.73	610.2	[M+H] ⁺	Quercetin 7-O-rutinoside	Flavonol
Mul0529	2.331194	0.001979	0.012244	4.083021	Negative	505.1	301.2	3.87	506.1	[M-H] ⁻	Quercetin O-acetylhexoside	Flavonol
Mul0516	0.935962	0.010116	0.030348	2.886952	Negative	463	301.1	3.68	464.096	[M-H] ⁻	Quercetin 3-O-glucoside (Isotrofolin)	Flavonol
Mul0239	0.612385	0.012174	0.034436	2.494541	Positive	465	302.9	4.04	464.096	[M+H] ⁺	Quercetin 4'-O-glucoside (Spiraeoside)	Flavonol
Mul0524	18.60429	0.000462	0.004726	1.710056	Negative	593.159	285.1	3.77	594.1585	[M-H] ⁻	Kaempferol 3-O-rutinoside (Nicotiflorin)	Flavonol
Mul0217	18.52576	0.003351	0.01543	1.648366	Positive	595.159	287	3.7	594.159	[M+H] ⁺	Kaempferol 3-O-robinobioside (Biorobin)	Flavonol
Mul0162	2.099913	0.000595	0.005521	1.051297	Positive	713.1	713.1	2.83	712.1	[M+H] ⁺	Quercetin 5-O-malonylhexosyl-hexoside	Flavonol
Mul0152	-0.92323	0.009675	0.02932	2.432712	Positive	627.1	430	2.65	626.1	[M+H] ⁺	8-C-hexosyl-hesperetin O-hexoside	Flavone C-glycosides
Mul0531	0.966193	0.007041	0.024038	3.014463	Negative	463.132	301.1	3.88	464.132	[M-H] ⁻	Hesperetin 5-O-glucoside	Flavanone
Mul0269	-3.02987	0.005179	0.020373	2.51429	Positive	273.1	137.1	5.3	272.069	[M+H] ⁺	Butein	Flavanone
Mul0233	18.64135	0.000578	0.005452	1.714918	Positive	611.19	303	3.99	610.19	[M+H] ⁺	Hesperetin 7-rutinoside (Hesperidin)	Flavanone
Mul0413	-1.46804	0.005017	0.019869	3.890246	Negative	191	85	1.22	192.063	[M-H] ⁻	Quinic acid	Quinate and its derivatives
Mul0445	-18.8981	0.001273	0.008792	1.871537	Negative	355.1	181.2	1.97	356.1	[M-H] ⁻	Homovanilloyl quinic acid	Quinate and its derivatives
Mul0508	0.609344	0.026779	0.057843	1.706714	Negative	337.1	190.9	3.44	338.1	[M-H] ⁻	3-O-p-Coumaroyl quinic acid	Quinate and its derivatives
Mul0215	8.723201	0.006962	0.023905	1.106944	Positive	321.1	147.5	3.68	320.1	[M+H] ⁺	5-O-p-Coumaroyl shikimic acid	Quinate and its derivatives
Mul0477	-1.49406	0.000295	0.004175	1.70672	Negative	341	179.1	2.62	342.132	[M-H] ⁻	Coniferin	Hydroxycinnamoyl derivatives
Mul0050	-1.51908	0.010674	0.031437	2.070708	Positive	138	137.9	0.8	137.048	[M+H] ⁺	Trigonelline	Alkaloids
Mul0074	2.505332	0.000351	0.004409	1.125143	Positive	86.1	56	1.17	85.1	[M+H] ⁺	Piperidine	Alkaloids
Mul0398	2.328446	0.001041	0.007728	1.739124	Negative	259	96.9	0.99	260.03	[M-H] ⁻	D-Glucose 6-phosphate	Carbohydrates
Mul0376	-1.62938	0.045979	0.084819	1.706329	Negative	179	70.9	0.77	180.063	[M-H] ⁻	D(+)-Glucose	Carbohydrates
Mul0149	1.124494	0.037024	0.072105	1.285352	Positive	341	179.1	2.58	340.079	[M+H] ⁺	Esculin (6,7-Dihydroxycoumarin-6-glucoside)	Coumarins
Mul0047	-1.16566	0.02939	0.062738	1.675012	Positive	256.2	124	0.8	255.2	[M+H] ⁺	Nicotinate ribonucleoside	Nicotinic acid derivatives
Mul0139	2.699733	0.001198	0.00847	1.064639	Positive	206.1	147.5	2.39	205.1	[M+H] ⁺	Methoxyindoleacetic acid	Indole derivatives
Mul0418	2.850806	6.09E-05	0.002413	4.913999	Negative	133	70.8	1.23	134.022	[M-H] ⁻	L(-)-Malic acid	Organic acids
Mul0427	1.976722	0.000151	0.002849	4.212903	Negative	117.03	99.9	1.31	118.027	[M-H] ⁻	Succinic acid	Organic acids
Mul0434	1.452999	0.000617	0.005637	3.189504	Negative	117.02	100	1.55	118.0266	[M-H] ⁻	Methylmalonic acid	Organic acids
Mul0025	2.64545	0.000146	0.002849	2.087319	Positive	132.1	86.2	0.75	131.1	[M+H] ⁺	5-Aminolevulinate	Organic acids
Mul0480	1.456675	0.000208	0.003195	2.061985	Negative	175.1	131.3	2.73	176.1	[M-H] ⁻	2-Isopropylmalate	Organic acids

Mul0450	0.757568	0.002087	0.012647	1.157112	Negative	131.042	86.9	2.15	132.0423	[M-H]-	2-Methylsuccinic acid	Organic acids
Mul0067	2.868755	0.000163	0.002942	1.080412	Positive	132.095	76.9	0.93	131.0946	[M+H]+	6-Aminocaproic acid	Organic acids
Mul0490	-2.75018	0.021653	0.050046	1.016282	Negative	137.03	92.5	2.98	138.032	[M-H]-	4-Hydroxybenzoic acid	Organic acids
Mul0318	3.636946	0.00021	0.003195	4.270911	Positive	520	125	8.08	519	[M+H]+	LysoPC 18:2 (2n isomer)	Lipids_Glycerophospholipids
Mul0315	-3.1916	0.001914	0.011966	3.59373	Positive	494.3	184.6	7.71	493.3	[M+H]+	LysoPC 16:1 (2n isomer)	Lipids_Glycerophospholipids
Mul0588	1.65101	0.021884	0.050382	3.436401	Negative	452	255.3	8.57	453	[M-H]-	LysoPE 16:0	Lipids_Glycerophospholipids
Mul0335	0.632806	0.018268	0.043405	3.032388	Positive	496.3	478.3	8.65	495.3	[M+H]+	LysoPC 16:0	Lipids_Glycerophospholipids
Mul0336	0.810786	0.016636	0.041004	3.004758	Positive	522.4	184.5	8.76	521.4	[M+H]+	LysoPC 18:1 (2n isomer)	Lipids_Glycerophospholipids
Mul0326	4.402583	0.002378	0.013324	2.416415	Positive	520.3	502.3	8.27	519.3	[M+H]+	LysoPC 18:2	Lipids_Glycerophospholipids
Mul0331	1.185721	0.032205	0.066888	1.739536	Positive	496.33	478.3	8.49	495.33	[M+H]+	LysoPC 16:0 (2n isomer)	Lipids_Glycerophospholipids
Mul0313	6.890017	0.015719	0.040483	1.430511	Positive	468.1	450.5	7.57	467.1	[M+H]+	LysoPC 14:0	Lipids_Glycerophospholipids
Mul0334	1.1438	0.017493	0.042068	1.32586	Positive	518.3	459.6	8.65	517.3	[M+H]+	LysoPC 18:3	Lipids_Glycerophospholipids
Mul0323	5.451924	0.001856	0.011853	1.149302	Positive	478.6	337.9	8.2	477.6	[M+H]+	LysoPE 18:2 (2n isomer)	Lipids_Glycerophospholipids
Mul0587	2.55955	0.013398	0.036175	1.144428	Negative	452.3	255.3	8.4	453.3	[M-H]-	LysoPE 16:0 (2n isomer)	Lipids_Glycerophospholipids
Mul0589	0.982282	0.014343	0.037866	1.045934	Negative	478.1	281.3	8.69	479.1	[M-H]-	LysoPE 18:1 (2n isomer)	Lipids_Glycerophospholipids
Mul0353	-1.79664	0.000416	0.004583	2.216916	Positive	353.2	261.8	9.91	352.2	[M+H]+	MAG (18:3) isomer1	Lipids_Glycerolipids
Mul0338	1.505818	0.011019	0.031928	2.215065	Positive	279.3	201.5	8.81	278.3	[M+H]+	Punicic acid	Lipids_Fatty acids
Mul0345	2.452674	0.014471	0.038034	2.01394	Positive	295.2	179.5	9.17	294.2	[M+H]+	9-Hydroxy-(10E,12Z,15Z)-octadecatrienoic acid	Lipids_Fatty acids
Mul0590	1.49988	0.012081	0.034436	1.855271	Negative	295	183.3	8.82	296	[M-H]-	9,10-EODE	Lipids_Fatty acids
Mul0544	-6.33719	0.000485	0.004886	5.19421	Negative	137	92.8	4.07	138.032	[M-H]-	Salicylic acid (SA)	Phytohormones
Mul0444	-5.59902	0.002288	0.013199	3.553304	Negative	299.1	137.2	1.96	300.1	[M-H]-	Salicylic acid O-glucoside	Phytohormones

Supplementary Table S4. Differentially accumulated metabolites between HG2 and BYW.

Index	log2_FC(case_mean/control_mean)	Pvalue	fdr	vip	Ion mode	Q1 (Da)	Q3 (Da)	Rt (min)	Molecular Weight (Da)	Ionization model	Compounds	Class
Mul0056	1.561504	0.000574	0.004732	2.898584	Positive	118.1	71.8	0.81	117.079	[M+H] ⁺	L-Valine	Amino acids
Mul0064	1.575115	0.000649	0.005004	2.802461	Positive	118	88	0.85	117.079	[M+H] ⁺	DL-Norvaline	Amino acids
Mul0092	0.4197	0.002011	0.009406	2.780579	Positive	132	85.9	1.23	131.0946	[M+H] ⁺	L-Isoleucine	Amino acids
Mul0097	0.362117	0.001691	0.008439	2.636583	Positive	132.1	86	1.27	131.0946	[M+H] ⁺	L-Leucine	Amino acids
Mul0367	2.026472	0.000274	0.00362	2.568908	Negative	131.054	71.8	0.75	132.054	[M-H] ⁻	L-Asparagine	Amino acids
Mul0374	1.561211	0.001238	0.00699	1.628287	Negative	132	99.9	0.77	133.0375	[M-H] ⁻	L-Aspartic acid	Amino acids
Mul0094	2.819428	8.37E-05	0.002106	3.840097	Positive	130	83.9	1.24	129.043	[M+H] ⁺	5-oxoproline	Amino acid derivatives
Mul0077	-6.71187	0.000565	0.004728	1.444157	Positive	308	162	1.18	307.084	[M+H] ⁺	Glutathione reduced form	Amino acid derivatives
Mul0443	-1.06751	0.029846	0.065576	1.484179	Negative	315.1	152.1	1.93	316.1	[M-H] ⁻	2,5-dihydroxy benzoic acid O-hexside	Benzoic acid derivatives
Mul0039	1.549138	0.000977	0.00652	2.304508	Positive	104.1	60.2	0.78	103.1	[M+H] ⁺	Choline	Cholines
Mul0140	-7.19485	0.005355	0.018698	2.99802	Positive	611.2	611.1	2.39	610.2	[M+H] ⁺	Gallocatechin-gallocatechin	Catechin derivatives
Mul0001	-0.29401	0.008255	0.025147	1.132749	Positive	203	112	0.54	202	[M+H] ⁺	Spermine	Phenolamines
Mul0120	0.720114	0.000236	0.003334	2.647598	Positive	167.1	121	1.95	166.1	[M+H] ⁺	6-Methylmercaptapurine	Nucleotide and its derivatives
Mul0084	2.254285	0.000555	0.004709	1.54097	Positive	136.1	136.1	1.21	135.0545	[M+H] ⁺	Adenine	Nucleotide and its derivatives
Mul0460	-4.35023	0.001593	0.008228	8.948604	Negative	465.1	285.3	2.41	466.1	[M-H] ⁻	Cyanidin O-syringic acid	Anthocyanins
Mul0145	-21.8716	1.85E-05	0.001761	4.929835	Positive	449.1	287.3	2.45	449.1	Protonated	Cyanidin 3-O-glucoside (Kuromanin)	Anthocyanins
Mul0150	-0.68824	0.007661	0.023658	2.668597	Positive	595	287.9	2.6	595	Protonated	Cyanidin 3-O-rutinoside (Keracyanin)	Anthocyanins
Mul0173	-4.97923	0.000233	0.003334	2.266757	Positive	463.123	301.4	3	463.123	Protonated	Peonidin O-hexoside	Anthocyanins
Mul0148	18.41852	0.016506	0.041722	1.407497	Positive	433.1	271	2.58	433.1	Protonated	Pelargonidin 3-O-beta-D-glucoside (Callistephin chloride)	Anthocyanins
Mul0530	7.709239	4.77E-07	0.000284	1.397094	Negative	503.1	341.3	3.88	504.1	[M-H] ⁻	Chrysoeriol O-acetylhexoside	Flavone
Mul0515	-1.91744	0.002114	0.009683	1.046573	Negative	521.1	329.3	3.68	522.1	[M-H] ⁻	Tricin O-saccharic acid	Flavone
Mul0529	7.511568	0.000805	0.005624	4.234331	Negative	505.1	301.2	3.87	506.1	[M-H] ⁻	Quercetin O-acetylhexoside	Flavonol
Mul0524	-2.82789	3.26E-05	0.001761	3.926413	Negative	593.159	285.1	3.77	594.1585	[M-H] ⁻	Kaempferol 3-O-rutinoside (Nicotiflorin)	Flavonol
Mul0516	-0.96147	0.000718	0.005199	3.870477	Negative	463	301.1	3.68	464.096	[M-H] ⁻	Quercetin 3-O-glucoside (Isotrifoliin)	Flavonol
Mul0217	-2.30053	0.000143	0.00266	3.052021	Positive	595.159	287	3.7	594.159	[M+H] ⁺	Kaempferol 3-O-robinobioside (Biorobin)	Flavonol
Mul0219	-0.62753	0.000894	0.006177	2.912885	Positive	611.2	303.7	3.73	610.2	[M+H] ⁺	Quercetin 7-O-rutinoside	Flavonol
Mul0201	-0.54884	0.012824	0.034783	2.669649	Positive	611.153	303	3.51	610.153	[M+H] ⁺	Quercetin 3-O-rutinoside (Rutin)	Flavonol
Mul0239	-0.36436	0.005761	0.01901	2.146034	Positive	465	302.9	4.04	464.096	[M+H] ⁺	Quercetin 4'-O-glucoside (Spiraeoside)	Flavonol
Mul0162	17.62822	0.000207	0.003185	1.128998	Positive	713.1	713.1	2.83	712.1	[M+H] ⁺	Quercetin 5-O-malonylhexosyl-hexoside	Flavonol
Mul0577	2.838234	0.011357	0.031921	1.049348	Negative	329.1	314.3	5.76	330.1	[M-H] ⁻	Di-O-methylquercetin	Flavonol
Mul0152	2.027396	0.000798	0.005624	2.126526	Positive	627.1	430	2.65	626.1	[M+H] ⁺	8-C-hexosyl-hesperetin O-hexoside	Flavone C-glycosides
Mul0501	-1.87475	0.003725	0.014184	1.666746	Negative	449.1	329.3	3.21	450.1	[M-H] ⁻	Eriodictyol C-hexoside	Flavone C-glycosides
Mul0212	-1.88469	0.000486	0.004374	1.503384	Positive	611.2	299.8	3.67	610.2	[M+H] ⁺	Luteolin 8-C-hexosyl-O-hexoside	Flavone C-glycosides
Mul0531	-0.87172	0.001026	0.006554	3.700161	Negative	463.132	301.1	3.88	464.132	[M-H] ⁻	Hesperetin 5-O-glucoside	Flavanone
Mul0233	-2.29821	0.000109	0.002407	3.18854	Positive	611.19	303	3.99	610.19	[M+H] ⁺	Hesperetin 7-rutinoside (Hesperidin)	Flavanone
Mul0260	-2.97923	0.012971	0.035021	2.221447	Positive	289.063	153.1	4.85	288.063	[M+H] ⁺	Eriodictyol	Flavanone
Mul0546	-3.24372	0.000293	0.003659	1.964797	Negative	609.2	301.3	4.09	610.19	[M-H] ⁻	Hesperetin 7-O-neohesperidoside (Neohesperidin)	Flavanone
Mul0413	-2.87014	0.006293	0.020097	6.796869	Negative	191	85	1.22	192.063	[M-H] ⁻	Quinic acid	Quinate and its derivatives
Mul0478	0.829689	0.042367	0.086482	2.062756	Negative	353.095	191.1	2.69	354.0951	[M-H] ⁻	Chlorogenic acid (3-O-Caffeoylquinic acid)	Quinate and its derivatives
Mul0456	0.239501	0.02939	0.065138	1.858831	Negative	353.1	191.1	2.21	354.095	[M-H] ⁻	1-O-Caffeoyl quinic acid	Quinate and its derivatives
Mul0215	9.119339	0.006949	0.021839	1.022803	Positive	321.1	147.5	3.68	320.1	[M+H] ⁺	5-O-p-Coumaroyl shikimic acid	Quinate and its derivatives
Mul0477	4.011197	0.001172	0.006922	1.133373	Negative	341	179.1	2.62	342.132	[M-H] ⁻	Coniferin	Hydroxycinnamoyl derivatives
Mul0110	-1.46409	0.001764	0.008618	3.138517	Positive	177	160.2	1.66	176.095	[M+H] ⁺	serotonin	Tryptamine derivatives
Mul0050	-1.15915	0.000406	0.00409	1.631196	Positive	138	137.9	0.8	137.048	[M+H] ⁺	Trigonelline	Alkaloids
Mul0379	0.73187	0.008483	0.025709	1.425679	Negative	341	58.8	0.78	342.1162	[M-H] ⁻	D-(+)-Sucrose	Carbohydrates
Mul0376	-0.89414	0.018312	0.045322	1.065684	Negative	179	70.9	0.77	180.063	[M-H] ⁻	D-(+)-Glucose	Carbohydrates
Mul0149	3.562936	0.001687	0.008439	1.70681	Positive	341	179.1	2.58	340.079	[M+H] ⁺	Esculin (6,7-Dihydroxycoumarin-6-glucoside)	Coumarins
Mul0047	-0.65315	0.000613	0.004921	1.139391	Positive	256.2	124	0.8	255.2	[M+H] ⁺	Nicotinate ribonucleoside	Nicotinic acid derivatives
Mul0418	21.86038	3.24E-05	0.001761	4.911363	Negative	133	70.8	1.23	134.022	[M-H] ⁻	L(-)-Malic acid	Organic acids
Mul0427	4.25887	0.000202	0.003185	4.391659	Negative	117.03	99.9	1.31	118.027	[M-H] ⁻	Succinic acid	Organic acids
Mul0386	-0.45621	0.016668	0.041953	2.398184	Negative	191	131	0.81	192.027	[M-H] ⁻	Citric acid	Organic acids
Mul0480	1.138898	8.06E-05	0.002106	1.781241	Negative	175.1	131.3	2.73	176.1	[M-H] ⁻	2-Isopropylmalate	Organic acids
Mul0025	1.526189	0.000131	0.00266	1.71567	Positive	132.1	86.2	0.75	131.1	[M+H] ⁺	5-Aminolevulinic acid	Organic acids
Mul0450	0.767389	0.000954	0.006517	1.08689	Negative	131.042	86.9	2.15	132.0423	[M-H] ⁻	2-Methylsuccinic acid	Organic acids
Mul0318	1.525641	0.027269	0.061355	3.112995	Positive	520	125	8.08	519	[M+H] ⁺	LysoPC 18:2 (2n isomer)	Lipids_Glycerophospholipids
Mul0326	2.087306	0.005734	0.01901	1.970729	Positive	520.3	502.3	8.27	519.3	[M+H] ⁺	LysoPC 18:2	Lipids_Glycerophospholipids
Mul0331	2.253607	0.010679	0.030643	1.946593	Positive	496.33	478.3	8.49	495.33	[M+H] ⁺	LysoPC 16:0 (2n isomer)	Lipids_Glycerophospholipids
Mul0587	2.583099	0.013124	0.035275	1.046758	Negative	452.3	255.3	8.4	453.3	[M-H] ⁻	LysoPE 16:0 (2n isomer)	Lipids_Glycerophospholipids
Mul0356	-1.41914	0.010944	0.031252	2.325112	Positive	355.1	337.9	10.36	354.1	[M+H] ⁺	MAG (18:2)	Lipids_Glycerolipids
Mul0287	-4.43296	0.044453	0.088905	2.248124	Positive	318.3	300.9	6.63	317.3	[M+H] ⁺	4-Hydroxysphinganine	Lipids_Fatty acids
Mul0338	0.79865	0.001247	0.00699	1.730812	Positive	279.3	201.5	8.81	278.3	[M+H] ⁺	Punicic acid	Lipids_Fatty acids
Mul0345	1.603234	0.022003	0.052489	1.687546	Positive	295.2	179.5	9.17	294.2	[M+H] ⁺	9-Hydroxy-(10E,12Z,15Z)-octadecatrienoic acid	Lipids_Fatty acids

Mul0590	1.033979	0.000513	0.004545	1.60706	Negative	295	183.3	8.82	296	[M-H]-	9,10-EODE	Lipids_Fatty acids
Mul0566	1.04875	0.020197	0.049371	1.005155	Negative	263	153.2	4.93	264.136	[M-H]-	(+)-cis,trans-Abscisic acid (ABA)	Phytohormones

Supplementary Table S5. Statistics of the sequencing reads for mulberry fruits.

Sequencing details	CS-1	CS-2	CS-3	HG2-1	HG2-2	HG2-3	BYW-1	BYW-2	BYW-3
Raw reads	46837546	45809226	45936772	45296040	48417824	50684876	46650630	46498720	57557936
Clean reads	45704960	44576292	44390454	44081086	46640874	49137728	44845108	45172650	56284532
Clean bases	6.27G	6.10G	6.06G	6.03G	6.36G	6.72G	6.11G	6.19G	7.72G
Q20 (%)	98.29	98.19	97.99	98.23	97.94	98.10	97.86	98.13	98.22
Q30 (%)	95.01	94.75	94.31	94.87	94.19	94.55	93.97	94.61	94.64
GC (%)	46.77	47.27	47.28	46.97	46.95	46.99	48.32	47.41	47.05

Supplementary Table S6. Structural genes involved in flavonoid metabolic pathway in mulberry fruits.

Function	Gene	Enzyme	KO id (EC no.)	No. All^a	No. Changed^b
Phenylpropanoid biosynthesis	<i>PAL</i>	Phenylalanine ammonia-lyase	k10775 (4.3.1.24)	6	6
	<i>C4H</i>	Trans-cinnamate 4-monooxygenase	k00487 (1.14.13.11)	4	3
	<i>4CL</i>	4-coumarate--CoA ligase	k01904 (6.2.1.12)	7	6
Anthocyanin biosynthesis	<i>CHS</i>	Chalcone synthase	K00660 (2.3.1.74)	7	6
	<i>CHI</i>	Chalcone isomerase	K01859 (5.5.1.6)	2	2
	<i>F3H</i>	Flavanone 3-hydroxylase	K00475 (1.14.11.9)	2	2
	<i>CYP75B1</i>	Flavonoid 3'-hydroxylase	K05280 (1.14.13.21)	1	1
	<i>CYP75B2</i>	Flavonoid 3'-hydroxylase	K05280 (1.14.13.21)	2	2
	<i>DFR</i>	Dihydroflavonol 4-reductase	K13082 (1.1.1.219)	1	1
	<i>ANS</i>	Anthocyanidin synthase	K05277 (1.14.11.19)	1	1
	<i>UFGT</i>	Anthocyanidin 3-O-glucosyltransferase	K12930 (2.4.1.115)	1	1
	<i>UGAT</i>	Cyanidin-3-O-glucoside 2"-O-glucuronosyltransferase	k12937 (2.4.1.254)	1	1
	<i>UGT75C1</i>	Anthocyanidin 3-O-glucoside 5-O-glucosyltransferase	K12338 (2.4.1. 298)	1	1
Flavone and flavonol biosynthesis	<i>FNS</i>	Flavone synthase	K13077 (1.14.11.22)	1	1
	<i>FLS</i>	Flavonol synthase	K05278 (1.14.11.23)	2	1
Flavanone biosynthesis	<i>LAR</i>	Leucoanthocyanidin reductase	K13081 (1.17.1.3)	1	1
	<i>ANR</i>	Anthocyanidin reductase	K08695 (1.3.1.77)	1	1

^a No. All, the total number of uni-transcripts analysed.

^b No.Changed, the number of uni-transcripts with expression significantly changed in fruits of Mulberry among the three cultivars.

Supplementary Table S7. Plant materials used in this study.

Abbreviation	Cultivars	Collection date	Collection place	Fruit color
CS	<i>Morus notabilis</i> C.K. Schneid	August	Ya'an City, Sichuan Province, China	Yellow-green color
HG2	<i>Morus alba</i> L. cv. Hongguo2	May	Beibei District, Chongqing City, China	Purple color
D10	<i>Morus alba</i> L. cv. Da10	May	Beibei District, Chongqing City, China	Purple color
BYW	<i>Morus alba</i> L. cv. Baiyuwang	June	Beibei District, Chongqing City, China	Oyster-white color
ZZB	<i>Morus alba</i> L. cv. Zhenzhubai	June	Beibei District, Chongqing City, China	White color
LJ109	<i>Morus alba</i> L. cv. Lunjiao109 (Monoecious)	May	Beibei District, Chongqing City, China	Red color
HGDBZZ	<i>Morus alba</i> L. cv. Hanguodabaizhenzhu	June	Beibei District, Chongqing City, China	Oyster-white color
F1-W	F1 population derived from LJ109 (male parent) and ZZB (female parent)	June	Beibei District, Chongqing City, China	White color
F1-Male	F1 population derived from LJ109 (male parent) and ZZB (female parent)	May	Beibei District, Chongqing City, China	No fruit, male tree
F2-P	F2 population derived from F1-W and F1-Male	May	Beibei District, Chongqing City, China	Red alternating with white
F2-R	F2 population derived from F1-W and F1-Male	May	Beibei District, Chongqing City, China	Red color
F2-W	F2 population derived from F1-W and F1-Male	June	Beibei District, Chongqing City, China	White color

Supplementary Table S8. Primers used in this work.

Primer Name	Forward primer	Reverse primer
Primers used for cloning candidate mulberry genes.		
<i>MYBA</i>	5'-ATGCAAACGGAGGGCTGTTC-3'	5'-CTACTGCATTTTCAGCATTTTCCT-3'
<i>TT2L1</i>	5'-ATGGGAAGAAACCCTTGTTGC-3'	5'-TTAATCAGTCAACCAGTTTTCTTCATCG-3'
<i>TT2L2</i>	5'-ATGGGAAGAAAACCTTGTTGTTCAA-3'	5'-TTAAACTTGAAGCCACCTATCGAAG-3'
<i>TT2L3</i>	5'-GATCTGGAGAGGGAGAGTGA-3'	5'-TTATAGGGCTAGAGTAAAGTCAATA-3'
<i>bHLH3</i>	5'-ATGTCTTGTCTTGATTTGACCTTCT-3'	5'-TCAATTATCGCTGTGGGGTAT-3'
<i>GL3</i>	5'-ATGGCTACTGGGCTCCAAAAC-3'	5'-TCAACTGTTCCAAGCAATTCTCTG-3'
<i>TTG1</i>	5'-AATTTTCCGTTATTCTGGCG-3'	5'-AGCAAGAAAAATAAAAATCAAAAAG-3'
<i>MYBF</i>	5'-ATGGGAAGAGCTCCGTGCT-3'	5'-TCAGGAGAGAAGCCAAGCGA-3'
<i>MYB4</i>	5'-ATGAACAAAGGAGCTTGGTCAA-3'	5'-TCATGTGAAGAGATTTTGAAGCGT-3'
<i>CYP75B1</i>	5'-ATGGCCTCTATCACCACCAT-3'	5'-TCAATATAAGTGTGGTCTAGTCT-3'
<i>CYP75B2</i>	5'-ATGCCCTCTATCTTACCATTCT-3'	5'-CTAAATTTTTGCTTCATATACATG-3'
<i>L484_012842</i>	5'-AGTAATTCATTATGGACTCCTCG-3'	5'-ATTTACACAAACAATCACCACACAT-3'
Primers for cell-feeding assays in yeast		
<i>CYP75B-pYES2</i>	5'-accgagctcgatccATGGCCTCTATCACCACCAT-3'	5'-agatgcatgctcgagTCAATATAAGTGTGGTCTAGTCT-3'
<i>CYP75B2-pYES2</i>	5'-accgagctcgatccATGCCCTCTATCTTACCATTCT-3'	5'-agatgcatgctcgagCTAAATTTTTGCTTCATATACATG-3'
<i>L484_012842-pYES2</i>	5'-accgagctcgatccATGGACTCCTCGTCGTCGT-3'	5'-agatgcatgctcgagTCACCACACATCACGTAGATACCT-3'
Primers for dual-luciferase reporter and transient color assays		
<i>CHS2P-LUC</i>	5'-ggtatcgataagcttGTCTGAAAACAGGAGTCGGA-3'	5'-agaactagtggatccTTTCAAAGAATTCACCGAGGATCT-3'
<i>CHIP-LUC</i>	5'-ggtatcgataagcttGTAGCCTCATTTTCGTCCTTT-3'	5'-agaactagtggatccTTGGGTTTCGGTTTTTGTGTA-3'
<i>FNSIP-LUC</i>	5'-ggtatcgataagcttTACGCAATTTTATACAAATCGAC-3'	5'-agaactagtggatccTTATTACTTGTCTGTAAGATGTCAAAT-3'
<i>CYP75B1P-LUC</i>	5'-ggtatcgataagcttAAATTTCTTGCACGCAATTA-3'	5'-agaactagtggatccAAGATAAAAGAGTTTCTGGAAGC-3'
<i>CYP75B2P-LUC</i>	5'-ggtatcgataagcttTTTGGGCAAAGCAGGGACTA-3'	5'-agaactagtggatccTGTGCTGTCTATGTTTTGTTTTTTT-3'
<i>FLSIP-LUC</i>	5'-ggtatcgataagcttGAATCAGCGAACTAAACGGG-3'	5'-agaactagtggatccGTTGTCTACTTAGCTAGCTAGATATCTT-3'
<i>FLS3P-LUC</i>	5'-ggtatcgataagcttTTTGAAGAACGCATAAAGGTC-3'	5'-agaactagtggatccGGCTACCAATAAGTTAAAGCTAG-3'
<i>DFRP-LUC</i>	5'-ggtatcgataagcttTAGCTAACGGTACGTTTGGTAGTGA-3'	5'-agaactagtggatccATTGCTGCTAATCTTTTGAAGACA-3'
<i>LARP-LUC</i>	5'-ggtatcgataagcttTTTAGTCGACGTTGTGAGAGTATG-3'	5'-agaactagtggatccGTTTGTCTTTTTTTTTTTTTTTTTT-3'
<i>ANRP-LUC</i>	5'-ggtatcgataagcttCATATTTGACGTTAAGCCTCTACG-3'	5'-agaactagtggatccGGCTATTGGATTCTTATTTCTTTT-3'
<i>ANSP-LUC</i>	5'-ggtatcgataagcttTTGAAACAAGGAGGGTTAAACTCA-3'	5'-agaactagtggatccATTAGCCTAATTTGTACCCTACTTTTC-3'
<i>UFGTP-LUC</i>	5'-ggtatcgataagcttATGTTTGTCTCATTTCTCGTA-3'	5'-agaactagtggatccGGTAAGTTTGTATGGAGGT-3'
<i>MYB4P-LUC</i>	5'-ggtatcgataagcttGCTTGAATTACTTTTGTGCGTGTG-3'	5'-agaactagtggatccTTCTCGCTTCTCACAGCAAGG-3'
<i>MYBA-SK</i>	5'-agaactagtggatccATGCAAACGGAGGGCTGTTC-3'	5'-taccgaattggtaccCTACTGCATTTTCAGCATTTTCCT-3'
<i>TT2L1-SK</i>	5'-agaactagtggatccATGGGAAGAAACCCTTGTTGC-3'	5'-taccgaattggtaccTTAATCAGTCAACCAGTTTTCTTCATCG-3'
<i>TT2L2-SK</i>	5'-agaactagtggatccATGGGAAGAAAACCTTGTTGTTCAA-3'	5'-taccgaattggtaccTTAAACTTGAAGCCACCTATCGAAG-3'
<i>TT2L3-SK</i>	5'-agaactagtggatccATGGGAGAGAGACGTCCTCG-3'	5'-taccgaattggtaccTCAATATTGTTGATCAGGAAAGGT-3'
<i>bHLH3-SK</i>	5'-agaactagtggatccATGTCTTGTCTTGATTTGACCTTCT-3'	5'-taccgaattggtaccTCAATTATCGCTGTGGGGTAT-3'
<i>GL3-SK</i>	5'-agaactagtggatccATGGCTACTGGGCTCCAAAAC-3'	5'-taccgaattggtaccTCAACTGTTCCAAGCAATTCTCTG-3'
<i>TTG1-SK</i>	5'-agaactagtggatccATGGAGAACACGACACAAGAATC-3'	5'-taccgaattggtaccTCAAACCTTTCAAAGCTGCATTT-3'
<i>MYBF-SK</i>	5'-agaactagtggatccATGGGAAGAGCTCCGTGCT-3'	5'-taccgaattggtaccTCAGGAGAGAAGCCAAGCGA-3'
<i>MYB4-SK</i>	5'-agaactagtggatccATGAACAAAGGAGCTTGGTCAA-3'	5'-taccgaattggtaccTCATGTGAAGAGATTTTGAAGCGT-3'
Primers for Y1H, Y2H and Y3H assays.		
<i>MYBA-AD</i>	5'-gattacgctcatatgCAAACGGAGGGCTGTTC-3'	5'-catctgcagctcgagCTACTGCATTTTCAGCATTTTCCT-3'
<i>TT2L1-AD</i>	5'-gattacgctcatatgGGAAGAAACCCTTGTTGC-3'	5'-catctgcagctcgagTTAATCAGTCAACCAGTTTTCTTCATCG-3'
<i>TT2L2-AD</i>	5'-gattacgctcatatgGGAAGAAAACCTTGTTGTTCAA-3'	5'-catctgcagctcgagTTAAACTTGAAGCCACCTATCGAAG-3'
<i>TT2L3-AD</i>	5'-gattacgctcatatgGGAGAGAGACGTCCTCG-3'	5'-tcatctgcagctcgagTCAATATTGTTGATCAGGAAAGGT-3'
<i>TTG1-AD</i>	5'-gattacgctcatatgGAGAACACGACACAAGAATC-3'	5'-catctgcagctcgagTCAAACCTTTCAAAGCTGCATTT-3'
<i>MYBF-AD</i>	5'-gattacgctcatatgGGAAGAGCTCCGTGCT-3'	5'-catctgcagctcgagTCAGGAGAGAAGCCAAGCGA-3'
<i>MYB4-AD</i>	5'-gattacgctcatatgAACAAAGGAGCTTGGTCAA-3'	5'-catctgcagctcgagTCATGTGAAGAGATTTTGAAGCGT-3'
<i>MYBA-BK</i>	5'-gaggacctgcatatgCAAACGGAGGGCTGTTC-3'	5'-caggtcgacggatccCTACTGCATTTTCAGCATTTTCCT-3'
<i>TT2L1-BK</i>	5'-gaggacctgcatatgGGAAGAAACCCTTGTTGC-3'	5'-caggtcgacggatccTTAATCAGTCAACCAGTTTTCTTCATCG-3'
<i>TT2L2-BK</i>	5'-gaggacctgcatatgGGAAGAAAACCTTGTTGTTCAA-3'	5'-caggtcgacggatccTTAAACTTGAAGCCACCTATCGAAG-3'
<i>TT2L3-BK</i>	5'-gaggacctgcatatgGGAGAGAGACGTCCTCG-3'	5'-caggtcgacggatccTCAATATTGTTGATCAGGAAAGGT-3'
<i>bHLH3-BK</i>	5'-gaggacctgcatatgTCTTGTCTTGATTTGACCTTCT-3'	5'-caggtcgacggatccTCAATTATCGCTGTGGGGTAT-3'
<i>GL3-BK</i>	5'-gaggacctgcatatgGCTACTGGGCTCCAAAAC-3'	5'-caggtcgacggatccTCAACTGTTCCAAGCAATTCTCTG-3'
<i>TTG1-BK</i>	5'-gaggacctgcatatgGAGAACACGACACAAGAATC-3'	5'-caggtcgacggatccTCAAACCTTTCAAAGCTGCATTT-3'
<i>MYBF-BK</i>	5'-gaggacctgcatatgGGAAGAGCTCCGTGCT-3'	5'-caggtcgacggatccTCAGGAGAGAAGCCAAGCGA-3'
<i>MYB4-BK</i>	5'-gaggacctgcatatgAACAAAGGAGCTTGGTCAA-3'	5'-caggtcgacggatccTCATGTGAAGAGATTTTGAAGCGT-3'
<i>ANSP-pBait</i>	5'-GGGGTACCTTGAAACAAGGAGGGTTAAACTCA-3'	5'-CCGCTCGAGATTAGCCTAATTTGTACCCTACTTTTC-3'
<i>LARP-pBait</i>	5'-GGGGTACCTTTAGTCGACGTTGTGAGAGTATG-3'	5'-CCGCTCGAGGTTTGTCTTTTTTTTTTTTTTTTTTTT-3'
<i>FLSIP-pBait</i>	5'-GGGGTACCGAATCAGCGAACTAAACGGG-3'	5'-CCGCTCGAGGTTGTCTACTTAGCTAGCTAGATATCTT-3'
<i>TTG1-pBridge</i>	5'-gtatcgccggaattcATGGAGAACACGACACAAGAATC-3'	5'-caggtcgacggatccTCAAACCTTTCAAAGCTGCATTT-3'
<i>bHLH3-pBridge</i>	5'-aaaggtggcggccgcaATGTCTTGTCTTGATTTGACCTTCT-3'	5'-tcagcccgaagatctTCAATTATCGCTGTGGGGTAT-3'
<i>GL3-pBridge</i>	5'-aaaggtggcggccgcaATGGCTACTGGGCTCCAAAAC-3'	5'-tcagcccgaagatctTCAACTGTTCCAAGCAATTCTCTG-3'
Primers for BiFC assays		

MYBA-BiFC 5'-gccactagtggatccATGCAAACGGAGGGCTGTTC-3' 5'-cccgggagcgggtaccCTGCATTTTCAGCATTTTCCT-3'
TT2L1-BiFC 5'-gccactagtggatccATGGGAAGAAACCCCTTGTTC-3' 5'-cccgggagcgggtaccATCAGTCAACCAGTTTTCTTCATCG-3'
TT2L2-BiFC 5'-gccactagtggatccATGGGAAGAAAACCTTGTTC-3' 5'-cccgggagcgggtaccAACTTGAAGCCACCTATCGAAG-3'
TT2L3-BiFC 5'-gccactagtggatccATGGGAGAGAGACGTCCTCG-3' 5'-cccgggagcgggtaccATATTGTTGATCAGGAAAGGT-3'
TTG1-BiFC 5'-gccactagtggatccATGGAGAACACGACACAAGAATC-3' 5'-cccgggagcgggtaccAACTTTCAAAGCTGCATTT-3'
MYB4-BiFC 5'-gccactagtggatccATGAACAAAGGAGCTTGGTCAA-3' 5'-cccgggagcgggtaccTCATGTGAAGAGATTTTGAAGCGT-3'
bHLH3-BiFC 5'-gccactagtggatccATGTCTTGTCTTGATTTGACCTTCT-3' 5'-cccgggagcgggtaccATTATCGCTGTGGGGTAT-3'
GL3-BiFC 5'-gccactagtggatccATGGCTACTGGGCTCCAAAAC-3' 5'-cccgggagcgggtaccACTGTTCCAAGCAATTCTCTG-3'

Primers for split luciferase complementation assays

MYBA-Nluc 5'-gacgagctcgggtaccATGCAAACGGAGGGCTGTTC-3' 5'-ccatttggatccCTGCATTTTCAGCATTTTCCT-3'
TT2L1-Nluc 5'-gacgagctcgggtaccATGGGAAGAAACCCCTTGTTC-3' 5'-ccatttggatccATCAGTCAACCAGTTTTCTTCATCG-3'
 5'-gacgagctcgggtaccATGGGAAGAAAACCTTGTTC-3'
TT2L2-Nluc 5'-gacgagctcgggtaccATGGGAGAGAGACGTCCTCG-3' 5'-ccatttggatccAACTTGAAGCCACCTATCGAAG-3'
TT2L3-Nluc 5'-gacgagctcgggtaccATGGAGAACACGACACAAGAATC-3' 5'-ccatttggatccATATTGTTGATCAGGAAAGGT-3'
TTG1-Nluc 5'-gacgagctcgggtaccATGGAGAACACGACACAAGAATC-3' 5'-ccatttggatccAACTTTCAAAGCTGCATTT-3'
MYB4-Nluc 5'-gacgagctcgggtaccATGAACAAAGGAGCTTGGTCAA-3' 5'-ccatttggatccTGTGAAGAGATTTTGAAGCGT-3'
bHLH3-Cluc 5'-tcccgggagcgggtaccATGTCTTGTCTTGATTTGACCTTCT-3' 5'-ccatttggatccTCAATTATCGCTGTGGGGTAT-3'
GL3-Cluc 5'-tcccgggagcgggtaccATGGCTACTGGGCTCCAAAAC-3' 5'-ccatttggatccTCAACTGTTCCAAGCAATTCTCTG-3'
TTG1-Cluc 5'-tcccgggagcgggtaccATGGAGAACACGACACAAGAATC-3' 5'-ccatttggatccTCAAACCTTTCAAAGCTGCATTT-3'

Primers for transient expression studies in tobacco.

5'-CGCGGATCCCATGTTGTGTGGACCTTTTTTATGTCC-3'
bHLH3P-GUS 3'
MYB4P-GUS 5'-CGCGGATCCGCTTGAATTACTTTTTGTGCGTGTG-3' 5'-CATGCCATGGTCTCACAAGCTGATCAGAGTTTCC-3'
 5'-CATGCCATGGTTCTCGCTTCTCACAGCAAGG-3'

Primers for subcellular localization (GFP) assays

MYBA-PZYG 5'-agaggacaggtaccATGCAAACGGAGGGCTGTTC-3' 5'-gacactagtggatccCTGCATTTTCAGCATTTTCCT-3'
TT2L1-PZYG 5'-agaggacaggtaccATGGGAAGAAACCCCTTGTTC-3' 5'-gacactagtggatccATCAGTCAACCAGTTTTCTTCATCG-3'
 5'-agaggacaggtaccATGGGAAGAAAACCTTGTTC-3'
TT2L2-PZYG 5'-agaggacaggtaccATGGGAGAGAGACGTCCTCG-3' 5'-gacactagtggatccAACTTGAAGCCACCTATCGAAG-3'
TT2L3-PZYG 5'-agaggacaggtaccATGGGAGAGAGACGTCCTCG-3' 5'-gacactagtggatccATATTGTTGATCAGGAAAGGT-3'
bHLH3-PZYG 5'-agaggacaggtaccATGTCTTGTCTTGATTTGACCTTCT-3' 5'-gacactagtggatccATTATCGCTGTGGGGTAT-3'
GL3-PZYG 5'-agaggacaggtaccATGGCTACTGGGCTCCAAAAC-3' 5'-gacactagtggatccACTGTTCCAAGCAATTCTCTG-3'
TTG1-PZYG 5'-agaggacaggtaccATGGAGAACACGACACAAGAATC-3' 5'-gacactagtggatccAACTTTCAAAGCTGCATTT-3'
MYBF-PZYG 5'-agaggacaggtaccATGGGAAGAGCTCCGTGCT-3' 5'-gacactagtggatccGGAGAGAAGCCAAGCGA-3'
MYB4-PZYG 5'-agaggacaggtaccATGAACAAAGGAGCTTGGTCAA-3' 5'-gacactagtggatccTGTGAAGAGATTTTGAAGCGT-3'

Primers for transformation of tobacco and Arabidopsis.

MYBA-PLGNL 5'-agaggacaggtaccATGCAAACGGAGGGCTGTTC-3' 5'-gacactagtggatccCTACTGCATTTTCAGCATTTTCCT-3'
 5'-gacactagtggatccTTAATCAGTCAACCAGTTTTCTTCATCG-3'
TT2L1-PLGNL 5'-agaggacaggtaccATGGGAAGAAACCCCTTGTTC-3' 5'-gacactagtggatccTTAAACTTGAAGCCACCTATCGAAG-3'
 5'-agaggacaggtaccATGGGAAGAAAACCTTGTTC-3' 5'-gacactagtggatccTCAATTATCGCTGTGGGGTAT-3'
TT2L2-PLGNL 5'-agaggacaggtaccATGTCTTGTCTTGATTTGACCTTCT-3' 5'-gacactagtggatccTCAACTGTTCCAAGCAATTCTCTG-3'
bHLH3-PLGNL 5'-agaggacaggtaccATGGCTACTGGGCTCCAAAAC-3' 5'-gacactagtggatccTCAAACCTTTCAAAGCTGCATTT-3'
GL3-PLGNL 5'-agaggacaggtaccATGGAGAACACGACACAAGAATC-3' 5'-gacactagtggatccTCAGGAGAGAAGCCAAGCGA-3'
TTG1-PLGNL 5'-agaggacaggtaccATGGGAAGAGCTCCGTGCT-3' 5'-gacactagtggatccTCATGTGAAGAGATTTTGAAGCGT-3'
MYBF-PLGNL 5'-agaggacaggtaccATGAACAAAGGAGCTTGGTCAA-3'

Primers for qRT-PCR and semi quantitative RT-PCR assays.

CHS2 5'-ATCATGGCAATCGGGACG-3' 5'-TGCTCACTGTTAGTAATACGGAAA-3'
CHI 5'-GGGAAGTCGGTGGAGGAA-3' 5'-CGTCTGCGTCAGTGAAATC-3'
F3H 5'-CGCCGTGCTGAGATTTG-3' 5'-CTAACCCTTACCCTGTA-3'
FNS 5'-CCCTCACCATCCTGCTC-3' 5'-GCTTTCGGCGGGCTTAT-3'
CYP75B1 5'-AATCAACGGCTACCACATCC-3' 5'-TCATACCCGCACAAATCCTAC-3'
CYP75B2 5'-TATCAATGGCTACCACATACCTAA-3' 5'-CCGACCCAAATGGAATCAC-3'
FLS1 5'-TTCCCGAGATACCCACCGTC-3' 5'-TTGGCGTAAACTCTTTCTCCT-3'
FLS3 5'-CATCCCTACCGAGGTCATACG-3' 5'-TTCTTTCCATTACGATCTTTTG-3'
DFR 5'-TTGTCGGACCGTAAAGATG-3' 5'-GCAGTGGGACCAAGAAAT-3'
LAR 5'-TTTGGGCACGACGTAGAC-3' 5'-GCCATCACCGTAGATTTTG-3'
ANS 5'-GCTTGCAGACCACATACTTT-3' 5'-TGCCGTCACCCATTTGC-3'
ANR 5'-GTGTCAAAGCGAAAACGG-3' 5'-CACAGGGTAGCCCCAAGTA-3'
UFGT 5'-GAGACGGGAGGGAGGTTAG-3' 5'-GGGTTCGTTTTCACTTCCTTTAG-3'
MYBA 5'-GAAGCCGGATGTCAAAG-3' 5'-TCCTACCCGCAATCAACG-3'
TT2L1 5'-GAATTACTGGAACACCAATTTAGG-3' 5'-TCTTATTGGACGGTGTATGCC-3'
TT2L2 5'-TCCTTGGAACAGATGGT-3' 5'-TGTTTCTTGTTGGCTTTG-3'
TT2L3 5'-CCGATGAAGGTTTCGAGTAGG-3' 5'-CTCCAGATTTCTTGAGTCCC-3'
bHLH3 5'-TCCAGTGGCTCTTAAATAACATC-3' 5'-AAGGCACAAGCGACCTCAAT-3'
GL3 5'-ACGGGATCATTTCTTAAATTATTCA-3' 5'-GTGAGAAAATAACAAGCTTCAACTGT-3'
TTG1 5'-GGCTCCGCAGAGTTACAGAC-3' 5'-AAAGGCGATGGCGATCCAAT-3'
MYBF 5'-TGTGAGAAAGTTGGGCTGAAG-3' 5'-CGGCATTCTTGGGTAGTGAT-3'
MYB4 5'-GGTCACGAGGTTTCAGATGGC-3' 5'-TTTTCCCGATTTGGGCTTTA-3'
MaActin 5'-GCATGAAGATCAAGGTGGTG-3' 5'-CATCTGCTGGAAGGTGCTAA-3'
NtActin 5'-TCACAGAAGCTCCTCCTAATCCA-3' 5'-GAGGGAAAGAAGCCTGAATG-3'
AtActin 5'-GCTCCTCTTAAACCAAAGGC-3' 5'-CACACCATCACCAGAATCCAGC-3'

Primers for transgene detection

MYB4P-GUS-check 5'-TCTTTAGCCTAAGTTTGCTGT-3'

5'-ACGCTGAGTAATTCGTTGAT-3'

The underline represents the restriction site;

Lower case letters: gene-specific primers with 15 bp extensions homologous to the ends of the linearized vector for In-Fusion cloning technology.

Supplemental Table S9. Accession numbers of sequences used in this study.

<i>Species</i>	<i>Sequence Name</i>	<i>Accession numbers</i>
<i>Antirrhinum majus</i>	AmDEL	AAA32663
<i>Arabidopsis thaliana</i>	AtCOP1	NP_180854.1
	AtEGL3	Q9CAD0
	AtGL3	NP_680372
	AtMYB11	NP_191820.1
	AtMYB111	NP_199744.1
	AtMYB113	NP_176811.1
	AtMYB12	NP_182268.1
	AtMYB3	NP_564176.2
	AtMYB4	NP_195574.1
	AtMYC1	Q8W2F1
	AtPAP1	NP_176057.1
	AtPAP2	NP_176813.1
	AtTT2	NP_198405.1
	AtTT8	Q9FT81
	AtTTG1	NP_001318637.1
<i>Brassica napus</i>	BnTTG1	XP_013643681.1
<i>Brassica oleracea var. botrytis</i>	BoTT8	ADP76654
	BoTTG1	XP_013599438.1
<i>Brassica rapa</i>	BrCOP1	VDC70492.1
	BrTTG1	XP_009150977.1
<i>Cajanus cajan</i>	CcCOP1	XP_020233903.1
<i>Diospyros kaki</i>	DkMYB2	AB503699.1
<i>Epimedium sagittatum</i>	EsMYBA1	KC335202
<i>Fragaria x ananassa</i>	FabHLH3	AFL02463
	FaMYB1	AF401220_1
	FaMYB11	AFL02461.1
<i>Fagopyrum tataricum</i>	FtMYB15;	KX758436
<i>Fragaria vesca subsp. vesca</i>	FvEGL1	XP_004308377
<i>Gossypium hirsutum</i>	GhCOP1L	XP_016696389.1
<i>Garcinia mangostana</i>	GmMYB10	ACM62751.1
<i>Gerbera hybrid cv. 'Terra Regina'</i>	GMYP10	AJ554700
<i>Gentiana triflora</i>	GtMYBP3	AB733016
	GtMYBP4	AB289446
<i>Hordeum vulgare subsp. Vulgare</i>	HvMYB10	AB645844
<i>Ipomoea nil</i>	InDEL	BAE94393
	InIVS	BAE94394
<i>Ipomoea purpurea</i>	InMYB1	AB232769
<i>Lilium hybrid division I</i>	LhbHLH1	BAE20057
	LhbHLH2	BAE20058
<i>Lotus japonicus</i>	LiTT8	AB490778
	LjGL3	AB492284
	LjTT2a	BAG12893.1
	LjTT2b	BAG12894
	LjTT2c	BAG12895
<i>Malus domestica</i>	MdbHLH3	ADL36597
	MdbHLH33	ABB84474
	MdMYB3	JN544704
	MdMYBA	AB279598
<i>Morella rubra</i>	MrMYB1	GQ340767
<i>Medicago truncatula</i>	MtMYB2	XM_003616340
<i>Perilla frutescens</i>	MYC-RP	AB024050
<i>Capsella rubella</i>	CrCOP1	XM_023784273.1
<i>Nicotiana tabacum</i>	NtAN1a	HQ589208
	NtAN1b	HQ589209
	NtJAF13	KF298397
<i>Pyrus communis</i>	PcMYB10	EU153575
<i>Perilla frutescens</i>	PfF3G1	AB103172
<i>Petunia x hybrida</i>	PhAN1	AAG25928
	PhAN11	AAC18914.1
	PhAN2	AAF66727.1
	PhJAF13	AAC39455
	PhMYB27	AHX24372
	PhMYB4	ADX33331.1
<i>Prunus persica</i>	PpMYB10	EU155160
	PpMYB18	KT159234
<i>Populus trichocarpa</i>	PtMYB134	FJ573151
	PtMYB165	XP_002315890.2
	PtMYB182	XP_002305872.1

<i>Ricinus communis</i>	RcCOP1	XP_002534127.1
<i>Raphanus sativus</i>	RsTT8	KY651179
	RsTTG1	XP_018484504.1
<i>Solanum tuberosum</i>	StAN1	JX848659
	StMTF1	EU310399
<i>Trifolium repens</i>	Tr-MYB134	KT699109
	Tr-MYB7	KT699107
<i>Vitis labrusca x Vitis vinifera</i>	VIMYBA1-1	AB073010
<i>Vitis vinifera</i>	VvMYB4a	ABL61515.1
	VvMYB4b	ACN94269.1
	VvMYBC1	ACC68685
	VvMYBC2-L1	AFX64995.1
	VvMYBC2-L2	ACX50288.2
	VvMYBC2-L3	AIP98385.1
	VvMYBF1	GQ423422
	VvMYBPA2	EU919682
	VvMYCA1	ABM92332
<i>Zea mays</i>	ZmB	CAA40544
	ZmIN1	AAB03841
	ZmLC	P13526
	ZmMYB-IF35	AF521880
	ZmPAC1	NP_001310302.1
<i>Morus alba L. cv. 'hongguo2'</i>	bHLH3	MN337861
	GL3	MN337862
	MYB4	MN337865
	MYBA	MN337857
	MYBF	MN337864
	TT2L1	MN337859
	TT2L2	MN337858
	TT2L3	MN337860
	TTG1	MN337863
<i>Morus notabilis C.K. Schneid</i>	Morus24997	EXB39302.1
	Morus25446	EXC01078.1
	CYP75B1	EXC06425.1
	CYP75B2	EXC06424.1
<i>Allium cepa</i>	F3'H	AY541035.1
<i>Arabidopsis thaliana</i>	F3'H	AF271651.1
<i>Callistephus chinensis</i>	F3'5'H	AF313489
	F3'H	FJ216428.1
<i>Campanula medium</i>	F3'5'H	D14590.1
<i>Coptis japonica</i>	CYP80B2	AB025030.1
<i>Delphinium grandiflorum</i>	F3'5'H	AY856345.1
<i>Eschscholzia californica</i>	CYP80B1	AF014801.1
<i>Gentiana triflora</i>	F3'5'H	D85184.1
	F3'H	AB193313.1
<i>Gerbera hybrida</i>	F3'H	DQ218417
<i>Glycine max</i>	F3'H	AF499731.1
	F3'5'H	AY117551.1
<i>Gossypium hirsutum</i>	F3'5'H	AY275430.1
<i>Hieracium pilosella</i>	F3'H	DQ319866
<i>Ipomoea nil</i>	F3'H	AB113264.1
<i>Lycianthes rantonneti</i>	F3'5'H	AF313490.1
<i>Matthiola incana</i>	F3'H	AF313491.1
<i>Nierembergia sp.</i>	F3'5'H	AB078514.1
<i>Osteospermum hybrida</i>	F3'5'H	KP899545
	F3'H	DQ250711
<i>Oryza sativa</i>	F3'H	XP_015613041.1
	F3'Hb	AK070442
<i>Pelargonium hortorum</i>	F3'H	AF315465.1
<i>Pericallis cruenta</i>	F3'5'H	AY791885
<i>Perilla frutescens</i>	F3'H	AB045593.1
<i>Petunia x hybrida</i>	F3'H	AF155332.1
	F3'5'H	AY245545.1
<i>Solanum melongena</i>	F3'5'H	X70824.1
<i>Solanum tuberosum</i>	F3'5'H	AY675559.1
<i>Torenia hybrida</i>	F3'5'H	AB012925.1
	F3'H	AB057673.1
<i>Vinca major</i>	F3'5'H	AB078781.1

Supplemental Table S10. Transcription factors correlated with *bHLH3* expression in connection network

ID in				
MorusDB	Family	Symbol	Description	Correlation
L484_012139	bZIP	BZIP61	Transcription factor RF2b [Morus notabilis]	Positive correlation
L484_020313	MYB_related	-	PREDICTED: protein RADIALIS-like 4 [Theobroma cacao]	Positive correlation
L484_022975	MYB	-	MYB4 [Morus notabilis]	Positive correlation
L484_020177	ERF	ERF012	Ethylene-responsive transcription factor [Morus notabilis]	Positive correlation
L484_019376	bHLH	ORG2	Transcription factor ORG2 [Morus notabilis]	Positive correlation
L484_013609	ZF-HD	-	Mini zinc finger 2 isoform 2, partial [Theobroma cacao]	Positive correlation
L484_014404	S1Fa-like	S1FA1	DNA-binding protein S1FA1 [Morus notabilis]	Positive correlation
L484_016991	C2H2	-	Transcriptional regulator TAC1 [Morus notabilis]	Positive correlation
L484_001828	Dof	DOF1.2	Dof zinc finger protein [Morus notabilis]	Positive correlation
L484_003860	WRKY	WRKY44	WRKY transcription factor 44 [Morus notabilis]	Positive correlation
L484_026215	HD-ZIP	GL2	Homeobox-leucine zipper protein GLABRA 2 [Morus notabilis]	Positive correlation
L484_000097	MYB	-	Transcription factor [Morus notabilis]	Positive correlation
L484_004072	TALE	-	Homeobox protein [Morus notabilis]	Positive correlation
L484_009669	DBB	-	Zinc finger protein CONSTANS-LIKE 2 [Morus notabilis]	Negative correlation
L484_023484	LBD	LBD11	lateral organ boundaries domain protein [Boehmeria nivea]	Positive correlation
L484_012905	MYB_related	ETC1	PREDICTED: MYB-like transcription factor ETC1 [Eucalyptus grandis]	Positive correlation
L484_007959	MIKC	-	Floral homeotic protein DEFICIENS [Morus notabilis]	Positive correlation
L484_017595	MYB_related	-	TRIPTYCHO (TRY) [Arabidopsis thaliana]	Positive correlation
L484_001405	M-type	-	PREDICTED: transcription factor of morphogenesis MCM1-like [Ziziphus jujuba]	Positive correlation
L484_004404	AP2	-	AP2-like ethylene-responsive transcription factor [Morus notabilis]	Positive correlation
L484_006971	B3	-	PREDICTED: auxin response factor 16-like [Citrus sinensis]	Positive correlation
L484_020870	YABBY	-	YABBY protein [Corchorus olitorius]	Positive correlation
L484_018706	MYB	-	Transcription factor [Morus notabilis]	Positive correlation
L484_027360	MYB	C1	Anthocyanin regulatory C1 protein [Morus notabilis]	Positive correlation
L484_015439	bHLH	BHLH75	PREDICTED: transcription factor bHLH75-like isoform X4 [Prunus mume]	Positive correlation
L484_016584	B3	-	B3 domain-containing transcription factor NGA4 [Morus notabilis]	Positive correlation
L484_021618	ERF	-	Ethylene-responsive transcription factor [Morus notabilis]	Positive correlation
L484_022665	MYB	MYB86	Transcription factor [Morus notabilis]	Positive correlation
L484_012134	NAC	-	NAC domain-containing protein 29 [Morus notabilis]	Positive correlation
L484_019377	bHLH	-	Transcription factor ORG2 [Morus notabilis]	Positive correlation
L484_019377	bHLH	-	Transcription factor ORG2 [Morus notabilis]	Positive correlation
L484_026077	bHLH	-	PREDICTED: transcription factor bHLH96-like [Glycine max]	Positive correlation
L484_006054	NAC	NAC072	NAC domain-containing protein 72 [Morus notabilis]	Negative correlation
L484_006652	C2H2	-	Zinc finger protein ZAT4 [Morus notabilis]	Positive correlation
L484_012750	HD-ZIP	-	Homeobox-leucine zipper protein ATHB-16 [Morus notabilis]	Positive correlation
L484_008831	NAC	NAC083	NAC domain-containing protein 29 [Morus notabilis]	Positive correlation