

Table S1. All detected metabolites in the berries of 'Red Globe' grape during postharvest senescence

Index	Q1 (Da)	Molecular Weight (Da)	Formula	Ionization model	Compounds	Class I	Class II	CAS	Level	RG0 1	RG0 2	RG0 3	RG12 1	RG12 2	RG12 3	RG24 1	RG24 2	RG24 3	mix01	mix02	mix03	cpd ID	kegg_map
mws4052	1.02E+02	1.01E+02	C4H7NO2	[M+H] ⁺	1-Aminocyclopropane-1-carboxylic acid	Others	Others	22059-21-8	B	6.71E+05	8.39E+05	5.30E+05	4.84E+05	7.37E+05	7.26E+05	4.07E+05	2.74E+05	4.20E+05	4.23E+05	4.98E+05	4.23E+05	C01234	ko00270,ko01100,ko01110
pme3011	1.04E+02	1.03E+02	C4H9NO2	[M+H] ⁺	γ -Aminobutyric acid	Organic acids	Organic acids	56-12-2	B	6.92E+06	7.24E+06	5.58E+06	7.42E+06	6.73E+06	6.49E+06	7.76E+06	7.31E+06	6.69E+06	6.04E+06	6.03E+06	6.05E+06	C00334	ko00250,ko00330,ko00410,ko00650,ko00760,ko01100
pme3017	1.04E+02	1.03E+02	C4H9NO2	[M+H] ⁺	Aminoisobutyric acid	Amino acids and derivatives	Amino acids and derivatives	62-57-7	B	1.69E+06	1.34E+06	1.25E+06	1.45E+06	1.33E+06	1.30E+06	1.41E+06	1.31E+06	1.51E+06	1.19E+06	1.24E+06	1.08E+06	C03665	--
pme3033	1.04E+02	1.03E+02	C4H9NO2	[M+H] ⁺	N,N-Dimethylglycine	Amino acids and derivatives	Amino acids and derivatives	1118-68-9	B	5.24E+06	5.55E+06	4.29E+06	4.80E+06	5.68E+06	4.90E+06	5.77E+06	5.32E+06	5.30E+06	4.35E+06	4.63E+06	4.05E+06	C01026	ko00260,ko01100
pmb0484	1.04E+02	1.03E+02	C5H13NO	[M+H] ⁺	Choline	Alkaloids	Alkaloids	62-49-7	B	1.70E+07	1.39E+07	1.27E+07	1.35E+07	1.35E+07	1.38E+07	1.55E+07	1.22E+07	1.45E+07	1.32E+07	1.28E+07	1.26E+07	C00114	ko00260,ko00564,ko01100,ko02010
mws0574	1.03E+02	1.04E+02	C4H8O3	[M-H] ⁻	α -Hydroxyisobutyric acid	Organic acids	Organic acids	594-61-6	A	6.84E+04	6.20E+04	5.31E+04	5.60E+04	5.36E+04	6.96E+04	6.86E+04	6.52E+04	5.30E+04	6.42E+04	5.69E+04	5.65E+04	--	--
pme2049	1.03E+02	1.04E+02	C4H8O3	[M-H] ⁻	2-Hydroxybutanoic acid	Organic acids	Organic acids	600-15-7	A	2.27E+05	1.87E+05	1.90E+05	1.85E+05	1.98E+05	2.35E+05	2.36E+05	2.32E+05	1.84E+05	2.15E+05	2.00E+05	2.13E+05	C05984	ko00640
mws0576	1.03E+02	1.04E+02	C4H8O3	[M-H] ⁻	3-Hydroxybutyrate	Organic acids	Organic acids	300-85-6	A	1.06E+05	7.06E+04	8.37E+04	8.73E+04	1.15E+05	9.21E+04	9.27E+04	9.83E+04	9.93E+04	1.02E+05	9.74E+04	9.23E+04	--	--
mws0890	1.04E+02	1.05E+02	C3H7NO3	[M-H] ⁻	D-Serine	Amino acids and derivatives	Amino acids and derivatives	312-84-5	A	4.55E+04	5.92E+04	6.10E+04	3.78E+04	4.57E+04	3.91E+04	3.36E+04	3.97E+04	4.27E+04	3.68E+04	4.81E+04	4.80E+04	--	--
pme2433	1.06E+02	1.05E+02	C4H11NO2	[M+H] ⁺	Diethanolamine	Others	Others	111-42-2	B	4.07E+05	2.07E+05	2.55E+05	2.82E+05	2.91E+05	2.36E+05	1.52E+05	1.25E+05	1.87E+05	1.77E+05	1.68E+05	1.78E+05	C06772	ko00564
mws0255	1.12E+02	1.11E+02	C4H5N3O	[M+H] ⁺	Cytosine	Nucleotides and derivatives	Nucleotides and derivatives	71-30-7	A	5.42E+04	4.31E+04	4.50E+04	4.23E+04	3.75E+04	4.60E+04	5.76E+04	4.77E+04	4.46E+04	4.36E+04	3.70E+04	4.27E+04	C00380	ko00240,ko01100
pme2122	1.12E+02	1.11E+02	C5H9N3	[M+H] ⁺	Histamine	Amino acids and derivatives	Amino acids and derivatives	51-45-6	B	4.52E+04	3.75E+04	4.44E+04	5.03E+04	6.14E+04	5.76E+04	5.17E+04	5.25E+04	5.04E+04	4.36E+04	5.41E+04	5.11E+04	C00388	ko00340,ko01100,ko01110
pme0257	1.11E+02	1.12E+02	C4H4N2O2	[M-H] ⁻	Uracil	Nucleotides and derivatives	Nucleotides and derivatives	66-22-8	A	1.36E+05	1.31E+05	1.40E+05	1.16E+05	1.40E+05	1.17E+05	1.10E+05	8.32E+04	1.07E+05	1.45E+05	1.32E+05	1.21E+05	C00106	ko00240,ko00410,ko00770,ko01100
pme0006	1.16E+02	1.15E+02	C5H9NO2	[M+H] ⁺	L-Proline	Amino acids and derivatives	Amino acids and derivatives	147-85-3	A	6.67E+06	6.07E+06	3.11E+06	9.83E+06	1.12E+07	9.55E+06	9.56E+06	1.14E+07	8.64E+06	7.87E+06	8.36E+06	7.88E+06	C00148	ko00970,ko01100,ko01230,ko02010
mws0256	1.18E+02	1.17E+02	C5H11NO2	[M+H] ⁺	L-Valine	Amino acids and derivatives	Amino acids and derivatives	72-18-4	A	6.30E+06	6.06E+06	4.10E+06	7.20E+06	7.94E+06	6.73E+06	6.74E+06	6.15E+06	6.50E+06	5.61E+06	5.26E+06	5.92E+06	C00183	ko00460,ko00770,ko00966,ko00970,ko01100,ko01110,ko01210,ko01230,ko02010
pme0120	1.18E+02	1.17E+02	C5H11NO2	[M+H] ⁺	5-Aminovaleric acid	Amino acids and derivatives	Amino acids and derivatives	660-88-8	B	1.46E+04	2.28E+04	1.79E+04	1.34E+05	2.72E+05	2.73E+05	2.28E+05	2.66E+05	3.21E+05	1.55E+05	1.61E+05	1.46E+05	C00431	ko00310,ko00330,ko01100
mws0191	1.18E+02	1.17E+02	C5H11NO2	[M+H] ⁺	Betaine	Alkaloids	Alkaloids	107-43-7	B	2.18E+05	2.53E+05	2.95E+05	1.96E+05	4.07E+05	3.37E+05	3.43E+05	3.70E+05	2.90E+05	2.59E+05	2.43E+05	2.31E+05	C00719	ko00260,ko01100,ko02010
mws0192	1.17E+02	1.18E+02	C4H6O4	[M-H] ⁻	Succinic acid	Organic acids	Organic acids	110-15-6	A	9.02E+06	1.23E+07	1.25E+07	1.25E+07	1.48E+07	1.36E+07	1.36E+07	1.64E+07	1.02E+07	1.35E+07	1.47E+07	1.38E+07	C00042	ko00250,ko00310,ko00350,ko00360,ko00620,ko00630,ko00640,ko00650,ko00760,ko00920,ko01100,ko01110,ko01200

mws0470	1.17E+02	1.18E+02	C4H6O4	[M-H]-	Methylmalonic acid	Organic acids	Organic acids	516-05-2	A	1.00E+07	1.28E+07	1.39E+07	1.34E+07	1.64E+07	1.36E+07	1.56E+07	1.92E+07	1.15E+07	1.45E+07	1.57E+07	1.53E+07	C02170	ko00240,ko00280,ko00640,ko01100
mws0147	1.17E+02	1.18E+02	C5H10O3	[M-H]-	3-Hydroxy-3-methyl butyric acid	Organic acids	Organic acids	625-08-1	B	1.94E+04	1.20E+04	9.37E+03	1.04E+04	2.27E+04	2.56E+04	1.24E+04	1.71E+04	1.12E+04	2.70E+04	1.37E+04	1.51E+04	--	--
mws0230	1.20E+02	1.19E+02	C4H9NO3	[M+H]+	L-(-)-Threonine	Amino acids and derivatives	Amino acids and derivatives	72-19-5	A	6.95E+06	6.06E+06	6.28E+06	7.05E+06	7.71E+06	6.05E+06	4.38E+06	3.81E+06	5.93E+06	4.34E+06	4.94E+06	4.39E+06	C00188	ko00290,ko00860,ko00970,ko01100,ko01110,ko01230,ko02010
mws0671	1.20E+02	1.19E+02	C4H9NO3	[M+H]+	L-Homoserine	Organic acids	Organic acids	672-15-1	B	7.69E+06	7.02E+06	5.14E+06	6.08E+06	6.59E+06	6.21E+06	3.70E+06	3.28E+06	4.62E+06	4.90E+06	3.72E+06	4.75E+06	C00263	ko00300,ko00920,ko01100,ko01110,ko01230
pmp001287	1.20E+02	1.19E+02	C8H9N	[M+H]+	N-Benzylmethyle isomethylamine	Alkaloids	Alkaloids	-	A	4.13E+06	6.93E+06	7.03E+06	5.29E+06	3.02E+06	5.34E+06	5.75E+06	4.79E+06	9.50E+06	5.75E+06	5.67E+06	5.86E+06	--	--
mws0491	1.22E+02	1.21E+02	C8H11N	[M+H]+	Phenethylamine	Others	Others	64-04-0	B	2.57E+04	6.50E+04	1.03E+05	2.68E+04	1.78E+04	2.74E+04	5.71E+04	8.08E+04	9.75E+04	5.28E+04	5.13E+04	5.27E+04	C05332	ko00360,ko01100
mws0133	1.23E+02	1.22E+02	C6H6N2O	[M+H]+	Nicotinamide	Others	Vitamin	98-92-0	B	1.62E+04	1.91E+04	2.48E+04	2.02E+04	1.76E+04	1.84E+04	1.66E+04	5.41E+04	2.09E+04	2.01E+04	2.23E+04	2.52E+04	C00153	ko00760,ko01100
pme0490	1.24E+02	1.23E+02	C6H5NO2	[M+H]+	Nicotinic acid	Others	Vitamin	59-67-6	B	3.43E+04	4.36E+04	9.30E+04	3.90E+04	3.37E+04	4.76E+04	3.60E+04	2.75E+04	4.37E+04	4.82E+04	4.59E+04	5.41E+04	C00253	ko00760,ko00960,ko01100,ko01110
mws0236	1.24E+02	1.25E+02	C2H7NO3S	[M-H]-	Aminoethanesulfonic acid	Organic acids	Organic acids	107-35-7	B	1.25E+04	1.09E+04	7.24E+03	5.96E+03	1.19E+04	1.22E+04	1.03E+04	1.22E+04	8.06E+03	8.33E+03	6.18E+03	8.90E+03	C00245	ko00430,ko00920,ko01100,ko02010
mws0813	1.28E+02	1.29E+02	C5H7NO3	[M-H]-	5-Oxoproline	Amino acids and derivatives	Amino acids and derivatives	149-87-1	B	1.04E+05	9.66E+04	7.93E+04	6.23E+04	6.55E+04	4.19E+04	4.75E+04	5.40E+04	5.08E+04	6.51E+04	6.80E+04	7.80E+04	C01879	ko00480,ko01100
mws0263	1.28E+02	1.29E+02	C5H7NO3	[M-H]-	L-Pyroglutamic acid	Amino acids and derivatives	Amino acids and derivatives	98-79-3	B	4.10E+04	3.78E+04	2.22E+04	1.46E+04	2.33E+04	1.17E+04	1.46E+04	2.27E+04	2.21E+04	2.17E+04	1.75E+04	2.16E+04	--	--
mws0345	1.28E+02	1.29E+02	C6H11NO2	[M-H]-	Pipecolic acid	Organic acids	Organic acids	535-75-1	B	5.65E+04	4.63E+04	3.00E+04	1.34E+04	3.72E+04	2.06E+04	1.78E+04	1.83E+04	1.40E+04	2.60E+04	2.37E+04	2.83E+04	--	--
Rfmb319	1.30E+02	1.29E+02	C6H11NO2	[M+H]+	Pipecolic acid	Amino acids and derivatives	Amino acids and derivatives	4043-87-2	A	4.10E+06	5.29E+06	4.67E+06	6.20E+06	4.54E+06	4.95E+06	4.85E+06	4.54E+06	5.42E+06	5.21E+06	5.04E+06	4.93E+06	--	--
mws0425	1.29E+02	1.30E+02	C5H6O4	[M-H]-	Citraconic acid	Organic acids	Organic acids	498-23-7	B	3.26E+05	3.58E+05	3.22E+05	6.53E+05	6.54E+05	5.87E+05	5.62E+05	5.12E+05	5.32E+05	5.55E+05	5.69E+05	5.71E+05	C02226	ko00290,ko00660,ko01100,ko01210
pme2693	1.31E+02	1.30E+02	C6H14N2O	[M+H]+	N-Acetylputrescine	Alkaloids	Alkaloids	18233-70-0	B	1.53E+04	2.61E+04	2.18E+04	2.23E+04	2.58E+04	1.90E+04	2.79E+04	3.97E+04	2.35E+04	1.63E+04	1.80E+04	2.15E+04	C02714	ko00330,ko01100
pmb0501	1.31E+02	1.30E+02	C5H14N4	[M+H]+	Agmatine	Alkaloids	Phenolamine	306-60-5	B	1.85E+04	2.55E+04	2.01E+04	2.94E+04	3.51E+04	2.28E+04	3.10E+04	4.47E+04	3.71E+04	2.38E+04	2.27E+04	2.69E+04	C00179	ko00330,ko01100
mws0712	1.30E+02	1.31E+02	C5H9NO3	[M-H]-	N-Propionylglycine	Amino acids and derivatives	Amino acids and derivatives	21709-90-0	B	3.54E+04	3.85E+04	3.18E+04	5.40E+04	6.08E+04	6.00E+04	6.03E+04	6.28E+04	4.86E+04	4.88E+04	4.57E+04	4.77E+04	--	--
mws0216	1.32E+02	1.31E+02	C5H9NO3	[M+H]+	Trans-4-Hydroxy-L-proline	Amino acids and derivatives	Amino acids and derivatives	51-35-4	B	6.72E+06	5.67E+06	3.41E+06	9.57E+06	9.34E+06	9.53E+06	1.23E+07	7.52E+06	9.60E+06	6.59E+06	6.37E+06	7.72E+06	C01157	ko00330,ko01100,ko02010
pme0274	1.32E+02	1.31E+02	C6H13NO2	[M+H]+	Aminocaproic acid	Organic acids	Organic acids	60-32-2	B	1.89E+07	1.66E+07	1.37E+07	2.14E+07	2.60E+07	2.18E+07	2.52E+07	2.28E+07	2.18E+07	1.95E+07	1.93E+07	2.01E+07	C02378	ko01100
pmp001198	1.32E+02	1.31E+02	C6H13NO2	[M+H]+	Deoxytagomine	Alkaloids	Alkaloids	197449-09-5	B	4.02E+06	3.77E+06	3.15E+06	5.02E+06	6.10E+06	5.03E+06	6.09E+06	5.18E+06	5.26E+06	4.58E+06	4.62E+06	4.30E+06	--	--
mws0258	1.32E+02	1.31E+02	C6H13NO2	[M+H]+	L-Isoleucine	Amino acids and derivatives	Amino acids and derivatives	73-32-5	A	1.17E+06	1.11E+06	9.16E+05	1.50E+06	1.78E+06	1.51E+06	1.64E+06	1.71E+06	1.53E+06	1.37E+06	1.34E+06	1.33E+06	C00407	ko00460,ko00960,ko00966,ko00970,ko01100,ko01110,ko01210,ko01230,ko02010
mws0227	1.32E+02	1.31E+02	C6H13NO2	[M+H]+	L-Leucine	Amino acids and derivatives	Amino acids and derivatives	61-90-5	A	1.20E+06	1.09E+06	8.88E+05	1.36E+06	1.70E+06	1.51E+06	1.57E+06	1.63E+06	1.42E+06	1.45E+06	1.25E+06	1.28E+06	C00123	ko00966,ko00970,ko01100,ko01110,ko01210,ko01230,ko02010

mws0473	1.31E+02	1.32E+02	C5H8O4	[M-H]-	2-Methylsuccinic acid	Organic acids	Organic acids	498-21-5	A	9.26E+05	1.01E+06	1.07E+06	1.01E+06	1.17E+06	1.19E+06	1.06E+06	1.25E+06	1.14E+06	1.21E+06	1.13E+06	1.13E+06	--	--
mws0001	1.33E+02	1.32E+02	C4H8N2O3	[M+H]+	L-Asparagine Anhydrous	Amino acids and derivatives	Amino acids and derivatives	70-47-3	B	1.80E+06	6.83E+05	6.53E+05	4.00E+06	4.12E+06	7.23E+06	2.32E+06	2.88E+06	2.97E+06	2.79E+06	2.28E+06	2.97E+06	C00152	ko00250,ko00460,ko00970,ko01100,ko01110,ko01230,ko00260,ko00261,ko00270,ko00300,ko00340,ko00410,ko00460,ko00710,ko00760,ko00770,ko00970,ko01100,ko01110,ko01200,ko01210,ko01230,ko02010
mws0219	1.32E+02	1.33E+02	C4H7NO4	[M-H]-	L-Aspartic Acid	Amino acids and derivatives	Amino acids and derivatives	56-84-8	B	7.01E+06	5.70E+06	4.52E+06	5.18E+06	4.52E+06	5.66E+06	2.12E+06	1.97E+06	3.07E+06	4.05E+06	4.09E+06	4.30E+06	C00049	ko02010
mws0275	1.33E+02	1.34E+02	C4H6O5	[M-H]-	L-(-)-Malic acid	Organic acids	Organic acids	636-61-3	A	3.45E+06	3.87E+06	3.83E+06	3.39E+06	3.16E+06	3.30E+06	3.16E+06	3.29E+06	3.48E+06	3.22E+06	3.18E+06	3.28E+06	C00497	ko00650,ko01100
pmb0374	1.36E+02	1.35E+02	C5H5N5	[M+H]+	Aminopurine	Alkaloids	Alkaloids	452-06-2	B	2.40E+04	2.07E+04	1.38E+04	1.78E+04	2.13E+04	1.56E+04	4.09E+04	3.77E+04	1.99E+04	2.44E+04	2.30E+04	2.23E+04	--	--
pme0040	1.36E+02	1.35E+02	C5H5N5	[M+H]+	Adenine	Nucleotides and derivatives	Nucleotides and derivatives	73-24-5	A	2.88E+05	3.33E+05	8.59E+05	3.34E+05	3.46E+05	2.97E+05	1.10E+06	9.03E+05	8.03E+05	5.77E+05	5.48E+05	5.40E+05	C00147	ko00230,ko00908,ko01100
mws0889	1.35E+02	1.36E+02	C4H8O5	[M-H]-	Threonate	Others	Others	6	B	7.00E+05	1.10E+06	9.16E+05	1.15E+06	1.04E+06	1.16E+06	1.36E+06	1.82E+06	9.31E+05	1.20E+06	1.17E+06	1.09E+06	--	--
pme1173	1.37E+02	1.36E+02	C5H4N4O	[M+H]+	Allopurinol	and derivatives	and derivatives	315-30-0	B	1.52E+04	9.23E+03	1.34E+04	9.00E+00	5.22E+03	9.00E+00	9.64E+03	9.39E+03	8.09E+03	7.15E+03	7.63E+03	8.15E+03	--	--
pme1738	1.38E+02	1.37E+02	C7H9N2O	[M+H]+	3-Carbamyl-1-methylpyridinium(1-Methylnicotinamide)	Others	Others	1005-24-9	A	2.29E+04	2.33E+04	1.81E+04	2.48E+04	1.47E+04	2.03E+04	1.81E+04	2.11E+04	2.47E+04	1.39E+04	1.62E+04	2.26E+04	C02918	ko00760,ko01100
mws0704	1.40E+02	1.41E+02	C2H8NO4P	[M-H]-	O-Phosphorylethanolamine	Others	Others	1071-23-4	B	7.26E+04	1.01E+05	6.89E+04	1.42E+05	1.42E+05	1.11E+05	1.47E+05	1.07E+05	1.65E+05	9.68E+04	1.23E+05	1.16E+05	--	--
Rfmb320	1.44E+02	1.43E+02	C7H13NO2	[M+H]+	1,2-N-Methylpipercolic acid	Amino acids and derivatives	Amino acids and derivatives	7730-87-2	B	1.94E+05	2.12E+05	1.57E+05	1.49E+05	2.18E+05	2.09E+05	1.97E+05	1.57E+05	1.77E+05	1.87E+05	2.04E+05	1.49E+05	--	--
Rfmb318	1.44E+02	1.44E+02	C7H14NO2+	[M]+	Proline βine(ProBet)	Amino acids and derivatives	Amino acids and derivatives	1195-94-4	B	9.45E+04	9.88E+04	8.04E+04	1.19E+05	1.06E+05	9.80E+04	9.58E+04	8.33E+04	9.34E+04	8.52E+04	9.31E+04	6.95E+04	--	--
mws0103	1.46E+02	1.45E+02	C9H7NO	[M+H]+	Indole-3-carboxaldehyde	Alkaloids	Plumerane	487-89-8	B	7.41E+03	1.20E+04	4.68E+03	8.48E+03	1.06E+04	7.51E+03	6.01E+03	2.38E+04	7.11E+03	1.13E+04	1.14E+04	9.70E+03	C08493	--
mws0567	1.46E+02	1.45E+02	C5H11N3O2	[M+H]+	Guanidinobutyric acid	Organic acids	Organic acids	463-00-3	B	3.10E+05	2.74E+05	4.67E+05	3.24E+05	4.72E+05	4.48E+05	1.65E+05	2.29E+05	5.93E+05	2.53E+05	2.78E+05	3.70E+05	C01035	ko00330,ko01100,ko00330,ko00410,ko00480,ko00940,ko01100,ko02010
mws0017	1.46E+02	1.45E+02	C7H19N3	[M+H]+	Spermidine	Alkaloids	Phenolamine	124-20-9	B	2.98E+04	3.03E+04	5.06E+04	5.13E+04	2.99E+04	2.42E+04	4.11E+04	2.23E+04	3.63E+04	3.93E+04	3.98E+04	4.19E+04	C00315	ko01100,ko02010
mws0208	1.45E+02	1.46E+02	C6H10O4	[M-H]-	Adipic Acid	Organic acids	Organic acids	124-04-9	B	6.03E+04	7.53E+04	6.83E+04	2.35E+04	3.59E+04	7.52E+04	3.06E+04	4.75E+04	4.60E+04	6.79E+04	5.20E+04	4.36E+04	C06104	ko01100
mws0924	1.45E+02	1.46E+02	C6H10O4	[M-H]-	2-Methylglutaric acid	Organic acids	Organic acids	617-62-9	B	5.55E+04	5.50E+04	5.75E+04	3.37E+04	3.08E+04	6.08E+04	3.61E+04	3.02E+04	4.80E+04	6.65E+04	4.58E+04	6.02E+04	--	--
pme0193	1.47E+02	1.46E+02	C5H10N2O3	[M+H]+	L-Glutamine	Amino acids and derivatives	Amino acids and derivatives	56-85-9	B	1.10E+05	9.91E+04	8.74E+04	1.51E+05	1.36E+05	1.37E+05	1.17E+05	1.32E+05	1.45E+05	1.17E+05	1.05E+05	1.02E+05	C00064	ko00220,ko00230,ko00240,ko00250,ko00630,ko00910,ko00970,ko01100,ko01230,ko02010

pme0026	1.47E+02	1.46E+02	C6H14N2 O2	[M+H] ⁺	L-(+)-Lysine	Amino acids and derivatives	Amino acids and derivatives	56-87-1	A	1.03E+05	9.06E+04	7.78E+04	1.50E+05	1.37E+05	1.20E+05	1.18E+05	1.27E+05	1.44E+05	1.13E+05	1.05E+05	1.13E+05	C00047	ko00300,ko00310, ko00780,ko00960, ko00970,ko01100, ko01110,ko01210, ko01230,ko02010
pme0014	1.48E+02	1.47E+02	C5H9NO4	[M+H] ⁺	L-Glutamic acid	Amino acids and derivatives	Amino acids and derivatives	56-86-0	B	7.85E+05	9.00E+05	4.33E+05	1.02E+06	7.58E+05	8.16E+05	5.30E+05	2.53E+05	3.56E+05	5.12E+05	5.15E+05	4.01E+05	C00025	ko00330,ko00332, ko00340,ko00430, ko00480,ko00630, ko00650,ko00660, ko00860,ko00910, ko00970,ko00998, ko01100,ko01110, ko01200,ko01210, ko01230,ko02010
mws1050	1.48E+02	1.47E+02	C5H9NO4	[M+H] ⁺	O-Acetyls erine Phthalic anhydride	Amino acids and derivatives	Amino acids and derivatives	5147-00-2	B	1.02E+05	1.56E+05	1.48E+05	7.52E+04	1.05E+05	1.10E+05	1.00E+05	1.26E+05	1.12E+05	1.15E+05	1.16E+05	1.14E+05	C00979	ko00920,ko00998, ko01100,ko01110, ko01200,ko01230, ko04122
pmp001285	1.49E+02	1.48E+02	C8H4O3	[M+H] ⁺		Phenolic acids	Phenolic acids	85-44-9	A	3.19E+05	4.73E+05	3.89E+05	6.81E+05	1.35E+06	6.51E+05	6.51E+05	7.88E+05	7.08E+05	5.58E+05	5.48E+05	5.93E+05	--	--
pme1210	1.50E+02	1.49E+02	C5H11NO 2S	[M+H] ⁺	L-Methionine 1-	Amino acids and derivatives	Amino acids and derivatives	63-68-3	A	3.28E+06	2.14E+06	1.65E+06	3.84E+06	6.33E+06	4.12E+06	4.76E+06	4.55E+06	3.84E+06	3.71E+06	3.42E+06	3.43E+06	C00073	ko00970,ko01100, ko01110,ko01210, ko01230
mws0847	1.50E+02	1.49E+02	C6H7N5	[M+H] ⁺	Methyladenine	Nucleotides and derivatives	Nucleotides and derivatives	5142-22-3	B	8.74E+04	6.66E+04	4.78E+04	1.00E+05	1.69E+05	1.15E+05	1.33E+05	1.16E+05	1.04E+05	1.01E+05	1.02E+05	9.35E+04	C02216	--
mws0262	1.49E+02	1.50E+02	C4H6O6	[M-H] ⁻	L-(+)-Tartaric acid	Organic acids	Organic acids	87-69-4	A	1.66E+06	1.69E+06	1.36E+06	1.81E+06	2.14E+06	1.81E+06	1.66E+06	1.89E+06	2.02E+06	1.95E+06	1.98E+06	1.81E+06	--	--
pme2019	1.49E+02	1.50E+02	C5H10O5	[M-H] ⁻	DL-Arabinose D-(-)- Arabinose	Others	and Alcohols Saccharides	147-81-9 10323-20- 3	A	1.18E+07	9.83E+06	9.40E+06	1.33E+07	1.40E+07	1.34E+07	1.16E+07	1.25E+07	1.15E+07	1.24E+07	1.23E+07	1.27E+07	--	--
mws1499	1.49E+02	1.50E+02	C5H10O5	[M-H] ⁻		Others	and Alcohols Saccharides		B	8.29E+06	6.65E+06	5.97E+06	8.34E+06	8.16E+06	9.78E+06	6.98E+06	7.49E+06	6.40E+06	7.26E+06	8.59E+06	8.39E+06	--	--
pme1109	1.52E+02	1.51E+02	C5H5N5O	[M+H] ⁺	Guanine	and derivatives	and derivatives	73-40-5	A	2.21E+04	2.74E+04	5.65E+04	2.04E+04	3.46E+04	1.98E+04	7.10E+04	8.08E+04	4.77E+04	3.49E+04	4.06E+04	3.21E+04	C00242	ko00230,ko01100
pme0183	1.52E+02	1.51E+02	C5H5N5O C5H4N4O	[M+H] ⁺	2-Hydroxy-6- aminopurine	Nucleotides and derivatives	Nucleotides and derivatives	3373-53-3	B	6.20E+04	6.16E+04	7.91E+04	8.23E+04	1.49E+05	1.44E+05	1.11E+05	1.89E+05	2.22E+05	1.39E+05	1.40E+05	1.11E+05	--	--
pme0256	1.51E+02	1.52E+02	C5H4N4O 2	[M-H] ⁻	Xanthine	Nucleotides and derivatives	Nucleotides and derivatives	69-89-6	B	1.07E+05	3.74E+04	2.96E+04	1.84E+05	4.17E+05	5.95E+05	7.93E+04	2.74E+05	1.59E+05	3.90E+05	2.49E+05	1.69E+05	C00385	ko00230,ko00232, ko01100,ko01110 ko00999,ko01100, ko01110
mws0458	1.51E+02	1.52E+02	C8H8O3	[M-H] ⁻	Vanillin	Phenolic acids	Phenolic acids	121-33-5	B	1.09E+04	1.65E+04	2.14E+04	3.35E+04	3.59E+04	2.12E+04	3.46E+04	3.48E+04	2.37E+04	2.06E+04	4.23E+04	3.11E+04	C00755	ko00040,ko01100, ko02010
mws0438	1.51E+02	1.52E+02	C5H12O5	[M-H] ⁻	L-Arabitol	Others	and Alcohols Saccharides	7643-75-6	B	8.37E+04	6.34E+04	5.92E+04	6.80E+04	7.99E+04	7.28E+04	7.75E+04	8.06E+04	7.31E+04	7.28E+04	7.00E+04	6.69E+04	--	--
pme0513	1.51E+02	1.52E+02	C5H12O5	[M-H] ⁻	Xylitol	Others	and Alcohols Saccharides	87-99-0	B	1.12E+05	6.12E+04	5.97E+04	9.10E+04	1.02E+05	9.02E+04	9.22E+04	8.16E+04	9.45E+04	8.70E+04	1.06E+05	7.38E+04	C00379	ko00040,ko01100, ko02010
mws0437	1.51E+02	1.52E+02	C5H12O5	[M-H] ⁻	D-Arabitol	Others	and Alcohols Saccharides	488-82-4	B	2.02E+04	1.87E+04	2.56E+04	1.51E+04	1.49E+04	1.46E+04	1.82E+04	1.58E+04	1.15E+04	1.45E+04	1.75E+04	2.01E+04	C01904	ko00040,ko01100
mws0213	1.51E+02	1.52E+02	C5H12O5	[M-H] ⁻	Ribitol	Others	and Alcohols	488-81-3	B	5.46E+04	4.69E+04	3.81E+04	4.89E+04	4.65E+04	4.17E+04	4.90E+04	4.64E+04	4.32E+04	4.55E+04	4.43E+04	4.06E+04	--	--
mws0183	1.53E+02	1.54E+02	C7H6O4	[M-H] ⁻	Protocatechuic acid	Flavonoids	Flavanols	99-50-3	B	9.79E+04	9.80E+04	1.54E+05	9.11E+04	6.42E+04	1.22E+05	4.83E+04	4.93E+04	7.93E+04	1.21E+05	8.82E+04	4.95E+04	C00230	ko00400,ko01100, ko01110
pmm001575	1.53E+02	1.54E+02	C7H6O4 C4H11O4	[M-H] ⁻	Gentisic acid Diethyl phosphate	Phenolic acids	Phenolic acids	490-79-9	B	2.59E+05	1.89E+05	3.37E+05	1.86E+05	2.44E+05	1.45E+05	1.43E+05	1.59E+05	1.62E+05	2.26E+05	2.03E+05	2.49E+05	C00628	ko00350,ko01100
pmb3099	1.53E+02	1.54E+02	C4H11O4 P	[M-H] ⁻		Organic acids	Organic acids	598-02-7	B	1.16E+05	1.32E+05	1.17E+05	1.32E+05	1.12E+05	1.40E+05	1.24E+05	1.18E+05	1.04E+05	9.29E+04	9.00E+04	8.19E+04	C06608	--
mws0254	1.56E+02	1.55E+02	C6H9N3O 2	[M+H] ⁺	L-Histidine DL-2- Aminoacidic acid	Amino acids and derivatives	Amino acids and derivatives	71-00-1	B	1.01E+07	9.43E+06	7.87E+06	1.11E+07	1.43E+07	1.07E+07	7.07E+06	8.85E+06	1.09E+07	9.85E+06	9.46E+06	9.46E+06	C00135	ko00970,ko01100, ko01110,ko01230, ko02010
mws1346	1.62E+02	1.61E+02	C6H11NO 4	[M+H] ⁺		Alkaloids	Alkaloids	542-32-5	B	2.32E+05	1.84E+05	2.07E+05	2.46E+05	1.66E+05	1.95E+05	1.83E+05	1.68E+05	1.87E+05	1.70E+05	1.79E+05	1.71E+05	--	--

pme3382	1.60E+02	1.61E+02	C6H11NO 4	[M-H]-	N-Acetylthreonine	Amino acids and derivatives	Amino acids and derivatives	17093-74- 2	B	2.24E+04	2.37E+04	2.93E+04	1.96E+04	2.67E+04	2.74E+04	2.30E+04	2.51E+04	2.65E+04	2.27E+04	2.44E+04	2.79E+04	--	--
pme2914	1.61E+02	1.62E+02	C6H10O5	[M-H]-	3-Hydroxy-3-methylpentane-1,5-dioic acid	Amino acids and derivatives	Amino acids and derivatives	503-49-1	A	7.01E+05	1.73E+06	1.66E+06	7.40E+05	4.65E+05	4.34E+05	4.23E+05	3.41E+05	9.09E+05	9.64E+05	9.68E+05	9.67E+05	C03761	--
pmf0440	1.63E+02	1.62E+02	C10H10O 2	[M+H]+	Methoxycinnamaldehyde	Phenolic acids	Phenolic acids	1963-36-6	B	1.02E+05	1.16E+05	1.01E+05	1.06E+05	1.06E+05	1.13E+05	1.10E+05	1.35E+05	1.03E+05	8.21E+04	7.67E+04	8.10E+04	--	--
pme2758	1.62E+02	1.63E+02	C5H9NO5	[M-H]-	4-Hydroxy-L-glutamic acid	Amino acids and derivatives	Amino acids and derivatives	3913-68-6	B	6.43E+04	4.58E+04	5.29E+04	4.56E+04	5.42E+04	4.78E+04	3.35E+04	3.35E+04	5.30E+04	4.45E+04	4.78E+04	4.21E+04	C03079	--
pmm001680	1.63E+02	1.64E+02	C9H8O3 C5H11NO	[M-H]-	Coumaric acid	Phenolic acids	Phenolic acids	500-05-0	A	2.50E+04	2.70E+04	1.77E+04	1.88E+04	2.78E+04	2.01E+04	2.29E+04	3.78E+04	3.46E+04	2.79E+04	2.51E+04	2.01E+04	--	--
pme2617	1.66E+02	1.65E+02	C5H11NO 3S	[M+H]+	Methionine sulfoxide	Amino acids and derivatives	Amino acids and derivatives	62697-73- 8	B	1.59E+06	1.73E+06	1.62E+06	1.63E+06	1.50E+06	1.75E+06	1.77E+06	1.69E+06	1.54E+06	1.76E+06	1.54E+06	1.63E+06	--	--
pme0021	1.66E+02	1.65E+02	C9H11NO 2	[M+H]+	L-Phenylalanine	Amino acids and derivatives	Amino acids and derivatives	63-91-2	A	5.68E+06	9.28E+06	9.31E+06	7.15E+06	4.11E+06	6.94E+06	7.79E+06	6.81E+06	1.19E+07	7.58E+06	7.83E+06	7.56E+06	C00079	ko00360,ko00400, ko00460,ko00940, ko00960,ko00966, ko00970,ko01100, ko01110,ko01210, ko01230,ko02010
pme0282	1.65E+02	1.66E+02	C8H6O4	[M-H]-	Phthalic acid	Organic acids	Organic acids	88-99-3	A	6.37E+04	8.49E+04	7.47E+04	1.00E+05	7.71E+04	8.00E+04	6.35E+04	8.99E+04	1.13E+05	8.19E+04	8.33E+04	8.07E+04	C01606	ko01100,ko02010
pme0281	1.65E+02	1.66E+02	C8H6O4	[M-H]-	Terephthalic acid	Phenolic acids	Phenolic acids	100-21-0	A	6.69E+05	2.69E+05	2.31E+05	9.40E+05	4.50E+05	2.43E+05	6.21E+05	6.35E+05	5.58E+05	5.02E+05	5.44E+05	5.20E+05	C06337	ko01100
mws0344	1.65E+02	1.66E+02	C5H10O6	[M-H]-	D-Xyloic acid	Organic acids	Organic acids	526-91-0	A	2.09E+07	2.80E+07	2.23E+07	2.48E+07	2.63E+07	2.50E+07	2.64E+07	3.48E+07	2.87E+07	2.77E+07	2.83E+07	2.97E+07	--	--
Hmbp001276	1.69E+02	1.68E+02	C8H8O4 C8H11NO	[M+H]+	Gallacetophenone	Others	Others	528-21-2	B	5.46E+05	1.56E+05	2.33E+05	2.32E+05	5.43E+05	2.91E+05	2.30E+05	2.38E+05	2.34E+05	3.01E+05	2.83E+05	3.53E+05	--	--
pme1383	1.70E+02	1.69E+02	C7H11N3 3	[M+H]+	Pyridoxine	Others	Vitamin	65-23-6	A	1.07E+06	1.36E+06	1.76E+06	7.12E+05	5.54E+05	6.40E+05	1.23E+06	8.00E+05	7.00E+05	9.37E+05	8.78E+05	9.16E+05	C00314	ko00750,ko01100
pme0181	1.70E+02	1.69E+02	C7H11N3 O2	[M+H]+	1-Methylhistidine	Amino acids and derivatives	Amino acids and derivatives	332-80-9	B	5.19E+04	3.01E+04	3.56E+04	4.04E+04	4.54E+04	2.85E+04	3.37E+04	4.79E+04	3.44E+04	4.92E+04	4.39E+04	3.81E+04	C01152	ko00340,ko01100
mws0279	1.70E+02	1.69E+02	C7H11N3 O2	[M+H]+	3-N-Methyl-L-histidine	Amino acids and derivatives	Amino acids and derivatives	368-16-1	B	1.81E+04	1.86E+04	1.53E+04	2.03E+04	2.31E+04	2.48E+04	2.25E+04	1.22E+04	1.25E+04	1.43E+04	1.31E+04	2.52E+04	--	--
mws0024	1.69E+02	1.70E+02	C7H6O5	[M-H]-	Gallic acid	Flavonoids	Flavanols	149-91-7	A	9.66E+03	1.10E+05	2.50E+04	2.05E+04	3.84E+04	2.61E+04	2.29E+04	3.04E+05	7.68E+04	5.57E+04	6.05E+04	5.49E+04	C01424	--
pme3009	1.75E+02	1.74E+02	C6H6O6	[M+H]+	Trans-Citric acid	Organic acids	Organic acids	4023-65-8	B	1.96E+06	1.73E+06	1.71E+06	2.15E+06	2.02E+06	2.19E+06	1.82E+06	1.86E+06	1.86E+06	1.79E+06	1.81E+06	2.02E+06	--	--
mws0154	1.73E+02	1.74E+02	C7H10O5 C7H14N2	[M-H]-	Shikimic acid	Organic acids	Organic acids	138-59-0	B	1.85E+04	5.38E+04	4.49E+04	2.12E+04	2.74E+04	2.64E+04	2.57E+04	3.00E+04	5.24E+04	3.13E+04	2.97E+04	2.82E+04	C00493	ko00400,ko01100, ko01110,ko01230
mws1401	1.75E+02	1.74E+02	C6H14N4 O3	[M+H]+	L-theanine	Amino acids and derivatives	Amino acids and derivatives	3081-61-6	B	7.89E+03	5.57E+03	5.17E+03	6.21E+03	1.08E+04	1.49E+04	7.80E+03	4.58E+03	3.85E+03	6.02E+03	5.32E+03	7.59E+03	C01047	--
mws0260	1.75E+02	1.74E+02	C6H14N4 O2	[M+H]+	L-(+)-Arginine	Amino acids and derivatives	Amino acids and derivatives	74-79-3	A	2.44E+06	2.53E+06	2.59E+06	2.61E+06	2.59E+06	2.63E+06	2.18E+06	2.35E+06	2.80E+06	2.36E+06	2.50E+06	2.20E+06	C00062	ko00220,ko00261, ko00330,ko00472, ko00970,ko00998, ko01100,ko01110, ko01230,ko02010
pme2559	1.74E+02	1.75E+02	C6H9NO5 C6H13N3	[M-H]-	N-Acetylaspartate	Amino acids and derivatives	Amino acids and derivatives	997-55-7	B	6.72E+04	6.13E+04	5.52E+04	5.53E+04	7.27E+04	6.06E+04	4.81E+04	6.12E+04	6.26E+04	6.11E+04	6.90E+04	7.23E+04	C01042	ko00250,ko01100
pme0008	1.76E+02	1.75E+02	C6H13N3 O3	[M+H]+	L-Citrulline	Amino acids and derivatives	Amino acids and derivatives	372-75-8	B	3.73E+06	3.04E+06	2.25E+06	1.75E+06	1.86E+06	1.99E+06	1.34E+06	1.73E+06	1.30E+06	1.49E+06	1.79E+06	2.10E+06	C00327	ko00220,ko01100, ko01110,ko01230
mws4175	1.75E+02	1.76E+02	C6H8O6	[M-H]-	D-Glucurono-6,3-lactone	Others	Others	32449-92- 6	B	2.14E+05	3.47E+05	3.00E+05	2.55E+05	1.94E+05	3.01E+05	4.49E+05	4.35E+05	3.05E+05	2.82E+05	3.00E+05	3.26E+05	--	--
Hmf00531	1.75E+02	1.76E+02	C6H8O6	[M-H]-	L-Ascorbic acid	Others	Vitamin	50-81-7	A	1.20E+04	1.03E+04	6.95E+03	1.01E+04	1.17E+04	8.58E+03	7.68E+03	1.85E+04	1.88E+04	1.58E+04	1.46E+04	1.42E+04	C00072	ko00053,ko00480, ko01100,ko01110
pme2253	1.77E+02	1.78E+02	C6H10O6	[M-H]-	L-Gulonic-γ-lactone	Others	and Alcohols	1128-23-0	B	8.57E+04	8.43E+04	8.96E+04	8.36E+04	9.40E+04	9.31E+04	1.04E+05	9.40E+04	8.41E+04	9.56E+04	7.84E+04	1.05E+05	C01040	ko00053,ko01100

mws1200	1.77E+02	1.78E+02	C10H10O3	[M-H]-	Trans-4-Hydroxycinnamic Acid Methyl Ester	Phenolic acids	Phenolic acids	19367-38-5	B	1.01E+03	2.10E+03	2.33E+03	5.59E+03	3.55E+03	3.13E+03	8.34E+03	1.71E+04	7.98E+03	5.66E+03	4.33E+03	5.70E+03	--	--
mws1195	1.79E+02	1.78E+02	C10H10O3	[M+H]+	Methyl p-coumarate	Phenolic acids	Phenolic acids	3943-97-3	B	9.00E+00	9.00E+00	9.00E+00	4.40E+03	5.62E+03	7.44E+03	8.16E+03	2.22E+04	9.10E+03	5.70E+03	4.50E+03	6.97E+03	--	--
mws0981	1.78E+02	1.79E+02	C6H5N5O2	[M-H]-	Isoxanthopterin	Nucleotides and derivatives	Nucleotides and derivatives	529-69-1	A	6.59E+03	8.08E+03	9.50E+03	1.43E+04	1.22E+04	1.09E+04	1.74E+04	1.71E+04	2.33E+04	1.32E+04	1.42E+04	1.17E+04	C03975	--
pme0516	1.79E+02	1.80E+02	C6H12O6	[M-H]-	Inositol	Others	Saccharides and Alcohols	87-89-8	B	2.59E+05	3.18E+05	3.48E+05	2.68E+05	1.91E+05	1.59E+05	2.43E+05	1.32E+05	2.31E+05	2.37E+05	2.06E+05	2.43E+05	C00137	ko00052,ko00053,ko00562,ko01100,ko02010,ko04070
mws4170	1.79E+02	1.80E+02	C6H12O6	[M-H]-	D-Glucose	Others	Saccharides and Alcohols	14431-43-7	A	3.18E+07	3.80E+07	3.41E+07	3.43E+07	3.34E+07	3.03E+07	3.88E+07	3.49E+07	3.16E+07	3.61E+07	3.55E+07	3.21E+07	--	--
mws0250	1.82E+02	1.81E+02	C9H11NO3	[M+H]+	L-(-)-Tyrosine	Amino acids and derivatives	Amino acids and derivatives	60-18-4	B	1.18E+07	1.21E+07	9.78E+06	1.01E+07	1.27E+07	8.50E+06	1.17E+07	1.06E+07	8.82E+06	1.04E+07	8.98E+06	1.03E+07	C00082	ko00350,ko00360,ko00400,ko00460,ko00730,ko00940,ko00950,ko00965,ko00966,ko00970,ko01100,ko01110,ko01210,ko01230
mws1350	1.81E+02	1.82E+02	C9H10O4	[M-H]-	Syringic Aldehyde	Phenolic acids	Phenolic acids	134-96-3	B	9.00E+00	9.00E+00	1.40E+04	9.00E+00	1.13E+04	7.14E+03	1.44E+04	2.05E+04	6.47E+03	9.92E+03	1.06E+04	1.18E+04	--	--
pme2237	1.81E+02	1.82E+02	C6H14O6	[M-H]-	Dulcitol	Others	Saccharides and Alcohols	608-66-2	B	2.84E+04	3.45E+04	3.50E+04	3.05E+04	3.70E+04	2.88E+04	4.07E+04	3.79E+04	3.41E+04	3.37E+04	3.98E+04	3.41E+04	C01697	ko00052,ko01100
pme2596	1.84E+02	1.83E+02	C8H9NO4	[M+H]+	4-Pyridoxic acid	Others	Vitamin	82-82-6	B	2.37E+04	1.35E+04	2.05E+04	9.57E+03	1.51E+04	2.00E+04	8.13E+03	1.32E+04	1.60E+04	1.14E+04	1.22E+04	1.22E+04	C00847	ko00750,ko01100,ko00260,ko00270,ko00970,ko00998,ko00999,ko01100,ko01200,ko01230
pme2602	1.84E+02	1.85E+02	C3H8NO6	[M-H]-	O-Phospho-L-serine	Amino acids and derivatives	Amino acids and derivatives	407-41-0	B	3.56E+04	2.85E+04	3.64E+04	2.29E+03	3.87E+03	3.23E+03	4.25E+03	1.26E+04	1.78E+04	1.15E+04	1.73E+04	1.15E+04	C01005	ko00350,ko00360,ko00400,ko00460,ko00730,ko00940,ko00950,ko00965,ko00966,ko00970,ko01100,ko01110,ko01210,ko01230
mws0752	1.85E+02	1.86E+02	C11H22O2	[M-H]-	Undecylic Acid	Lipids	Free fatty acids	112-37-8	B	3.28E+05	2.91E+05	3.30E+05	3.03E+05	3.35E+05	3.18E+05	3.10E+05	3.34E+05	3.17E+05	3.46E+05	3.35E+05	3.20E+05	--	--
pme0137	1.87E+02	1.88E+02	C7H12N2O4	[M-H]-	N-α-Acetyl-L-glutamine	Amino acids and derivatives	Amino acids and derivatives	2490-97-3	B	3.22E+05	4.58E+05	3.10E+05	4.08E+05	3.47E+05	3.45E+05	4.49E+05	5.89E+05	3.82E+05	3.25E+05	4.46E+05	4.38E+05	--	--
mws0237	1.87E+02	1.88E+02	C9H16O4	[M-H]-	Anchoic Acid	Organic acids	Organic acids	123-99-9	A	1.25E+05	1.27E+05	1.56E+05	1.53E+05	1.47E+05	1.46E+05	1.46E+05	1.81E+05	1.38E+05	1.53E+05	1.60E+05	1.51E+05	C08261	--
mws0736	1.89E+02	1.88E+02	C8H16N2O3	[M+H]+	N-Glycyl-L-leucine	Amino acids and derivatives	Amino acids and derivatives	869-19-2	B	1.63E+06	2.46E+06	6.71E+05	1.41E+06	2.14E+05	2.26E+06	9.28E+05	6.70E+05	9.25E+05	1.27E+06	1.35E+06	1.22E+06	C02155	--
pme0122	1.89E+02	1.88E+02	C8H16N2O3	[M+H]+	N6-Acetyl-L-lysine	Amino acids and derivatives	Amino acids and derivatives	692-04-6	B	2.88E+05	2.90E+05	3.16E+05	4.66E+05	3.91E+05	2.32E+05	3.93E+05	2.88E+05	4.64E+05	4.20E+05	3.07E+05	3.49E+05	C02727	ko00310,ko01100
pme3388	1.89E+02	1.88E+02	C7H16N4O2	[M+H]+	H-HomoArg-OH	Amino acids and derivatives	Amino acids and derivatives	156-86-5	B	6.11E+05	5.65E+05	4.36E+05	6.08E+05	6.22E+05	6.97E+05	5.61E+05	7.14E+05	7.36E+05	4.66E+05	4.74E+05	5.76E+05	C01924	--
mws0193	1.90E+02	1.89E+02	C7H15N3O3	[M+H]+	L-Homocitrulline	Amino acids and derivatives	Amino acids and derivatives	1190-49-4	B	2.54E+04	2.40E+04	2.00E+04	5.54E+04	2.17E+04	1.90E+04	1.97E+04	3.05E+04	2.21E+04	3.23E+04	2.83E+04	3.57E+04	C02427	--
mws0281	1.91E+02	1.92E+02	C6H8O7	[M-H]-	Citric Acid	Organic acids	Organic acids	77-92-9	A	1.87E+07	2.06E+07	1.97E+07	2.14E+07	2.40E+07	2.39E+07	2.89E+07	2.49E+07	2.23E+07	2.64E+07	2.32E+07	2.22E+07	C00158	ko00020,ko00250,ko00630,ko01100,ko01110,ko01200,ko01210,ko01230
mws0277	1.91E+02	1.92E+02	C7H12O6	[M-H]-	Kinic acid	Organic acids	Organic acids	77-95-2	B	4.48E+05	4.80E+05	6.05E+05	6.15E+05	5.45E+05	5.85E+05	6.25E+05	5.89E+05	4.75E+05	6.18E+05	6.53E+05	5.83E+05	C00296	ko00400,ko01100
mws1213	1.93E+02	1.94E+02	C6H10O7	[M-H]-	Aldehydo-D-galacturonate	Organic acids	Organic acids	685-73-4	A	2.52E+06	3.65E+06	3.30E+06	2.84E+06	2.24E+06	2.91E+06	4.67E+06	3.28E+06	2.66E+06	3.31E+06	3.47E+06	3.76E+06	--	--
pme3705	1.93E+02	1.94E+02	C6H10O7	[M-H]-	D-Glucuronic acid	Others	Saccharides and Alcohols	6556-12-3	A	2.50E+06	3.37E+06	2.90E+06	2.89E+06	2.27E+06	3.33E+06	4.51E+06	4.50E+06	3.51E+06	3.70E+06	3.67E+06	4.23E+06	C00191	ko00040,ko00053,ko00520,ko00562,ko01100
mws1189	1.93E+02	1.94E+02	C6H10O7	[M-H]-	D-Galacturonic acid(Gal A)	Organic acids	Organic acids	91510-62-2	B	2.14E+06	3.36E+06	3.16E+06	3.08E+06	2.17E+06	3.02E+06	4.60E+06	3.19E+06	3.41E+06	3.25E+06	3.53E+06	4.03E+06	C00333	ko00040,ko00053,ko00520,ko01100,ko02010

pme2266	2.45E+02	2.44E+02	C10H16N2O3S	[M+H] ⁺	Biotin	Others	Vitamin	58-85-5	B	4.68E+04	1.37E+05	1.12E+05	4.83E+04	4.43E+04	6.63E+04	3.11E+04	4.94E+04	7.97E+04	7.97E+04	6.72E+04	8.05E+04	C00120	ko00780,ko01100,ko02010
pme3961	2.52E+02	2.51E+02	C10H13N5O3	[M+H] ⁺	Deoxyadenosine	Nucleotides and derivatives	Nucleotides and derivatives	958-09-8	B	4.21E+03	6.13E+03	1.08E+04	8.36E+03	6.74E+03	5.94E+03	1.20E+04	1.93E+04	1.21E+04	7.83E+03	9.44E+03	1.09E+04	C00559	ko00230,ko01100,ko02010
pmm001578	2.55E+02	2.56E+02	C16H32O2	[M-H] ⁻	Hexadecanoic acid	Lipids	Free fatty acids	57-10-3	A	2.16E+07	2.32E+07	2.03E+07	1.79E+07	2.05E+07	1.70E+07	2.60E+07	2.60E+07	2.16E+07	1.53E+07	2.41E+07	2.27E+07	C00249	ko00071,ko00073,ko01040,ko01100,ko01212
mws0120	2.58E+02	2.57E+02	C8H20NO6P	[M+H] ⁺	Choline alfoscerate	Lipids	PC	28319-77-9	B	3.10E+05	2.25E+05	3.92E+05	1.66E+05	2.43E+05	2.75E+05	1.78E+05	1.46E+05	2.52E+05	2.09E+05	2.06E+05	2.09E+05	--	--
mws0866	2.59E+02	2.60E+02	C6H13O9P	[M-H] ⁻	D-Glucose 6-phosphate	Others	Saccharides	56-73-5	A	3.11E+06	2.67E+06	3.37E+06	1.65E+06	2.95E+06	2.05E+06	2.01E+06	1.65E+06	2.43E+06	2.16E+06	2.15E+06	1.99E+06	C00092	ko00500,ko00562,ko00998,ko01100
mws1090	2.59E+02	2.60E+02	C6H13O9P	[M-H] ⁻	Glucose-1-phosphate	Others	Saccharides and Alcohols	59-56-3	A	1.43E+06	2.25E+06	2.96E+06	1.45E+06	8.75E+05	3.30E+06	1.53E+06	1.70E+06	2.02E+06	1.53E+06	2.22E+06	2.37E+06	--	--
pme0230	2.68E+02	2.67E+02	C10H13N5O4	[M+H] ⁺	Adenosine 9-(β-D-Arabinofuranosyl)hypoxanthine	Nucleotides and derivatives	Nucleotides and derivatives	58-61-7	A	8.50E+05	1.62E+06	3.45E+06	1.19E+06	1.16E+06	1.22E+06	2.62E+06	2.99E+06	3.34E+06	2.28E+06	2.11E+06	2.13E+06	C00212	ko00230,ko01100,ko02010
mws1060	2.67E+02	2.68E+02	C10H12N4O5	[M-H] ⁻	1-Feruloyl-sn-glycerol	Nucleotides and derivatives	Nucleotides and derivatives	7013-16-3	B	5.55E+04	2.56E+04	3.22E+04	8.81E+03	1.23E+04	1.19E+04	4.26E+03	2.82E+04	2.32E+04	1.89E+04	2.59E+04	2.86E+04	--	--
pmp000086	2.69E+02	2.68E+02	C13H16O6	[M+H] ⁺	Cis-10-Heptadecenoic Acid	Phenolic acids	Phenolic acids	-	B	5.90E+04	1.88E+04	1.97E+04	2.19E+04	1.60E+04	2.06E+04	1.32E+04	1.79E+04	1.59E+04	1.88E+04	2.54E+04	2.00E+04	--	--
mws0383	2.67E+02	2.68E+02	C17H32O2	[M-H] ⁻	29743-97-3	Lipids	Free fatty acids	3	B	2.21E+04	3.61E+04	1.06E+05	2.29E+04	2.45E+04	2.18E+04	6.63E+04	8.42E+04	3.29E+04	4.96E+04	6.23E+04	5.75E+04	--	--
pme3475	2.73E+02	2.72E+02	C15H12O5	[M+H] ⁺	Butin	Flavonoids	Dihydroflavone	492-14-8	B	9.63E+03	9.06E+03	1.40E+04	1.36E+04	9.75E+03	5.90E+03	1.79E+04	2.87E+04	2.27E+04	2.09E+04	1.72E+04	2.01E+04	C09614	ko00941
pme0376	2.71E+02	2.72E+02	C15H12O5	[M-H] ⁻	Naringenin	Flavonoids	Dihydroflavone	480-41-1	B	7.37E+03	7.31E+03	1.43E+04	1.51E+04	6.40E+03	6.38E+03	1.48E+04	2.06E+04	1.88E+04	1.31E+04	1.45E+04	1.47E+04	C00509	ko00941,ko00943,ko01100,ko01110
mws0914	2.71E+02	2.72E+02	C15H12O5	[M-H] ⁻	Pinobanksin	Flavonoids	Dihydroflavono	548-82-3	A	5.56E+03	6.27E+03	1.24E+04	1.11E+04	7.48E+03	5.79E+03	1.66E+04	2.06E+04	1.72E+04	1.43E+04	1.34E+04	1.38E+04	C09826	ko00941
pmp001264	2.74E+02	2.73E+02	C16H35NO2	[M+H] ⁺	Hexadecylsphingosine	Lipids	Sphingolipids	-	A	2.16E+06	1.83E+06	2.48E+06	2.25E+06	1.96E+06	2.65E+06	2.42E+06	2.67E+06	2.19E+06	1.75E+06	1.85E+06	1.93E+06	--	--
mws1038	2.77E+02	2.78E+02	C11H22N2O4S	[M-H] ⁻	(R)-Pantetheine	Others	Others	496-65-1	A	7.70E+04	6.13E+04	6.38E+04	3.21E+04	1.56E+04	3.05E+04	1.01E+04	5.73E+03	9.00E+00	1.88E+04	4.19E+04	2.67E+04	C00831	ko00332,ko00770
mws5035	2.79E+02	2.78E+02	C15H22N2O3	[M+H] ⁺	Leucylphenylalanine	Amino acids and derivatives	Amino acids and derivatives	56217-82-4	B	6.07E+03	9.65E+03	2.42E+04	1.57E+04	1.04E+04	8.44E+03	2.77E+04	1.03E+04	1.38E+04	1.19E+04	1.32E+04	1.44E+04	--	--
mws0366	2.77E+02	2.78E+02	C18H30O2	[M-H] ⁻	γ-Linolenic Acid	Lipids	Free fatty acids	506-26-3	B	2.42E+06	2.39E+06	1.90E+06	1.28E+06	1.13E+06	1.27E+06	1.44E+06	1.41E+06	1.64E+06	1.82E+06	1.76E+06	1.71E+06	--	--
mws0629	2.81E+02	2.80E+02	C13H16N2O5	[M+H] ⁺	Asp-phe	Amino acids and derivatives	Amino acids and derivatives	13433-09-5	B	1.34E+05	1.52E+05	1.19E+05	1.56E+05	1.26E+05	1.49E+05	1.57E+05	1.49E+05	1.40E+05	1.54E+05	1.36E+05	1.63E+05	--	--
YC512118	2.82E+02	2.81E+02	C18H35NO	[M+H] ⁺	Octadecenoic amide	Others	Others	-	B	1.72E+05	1.28E+05	1.39E+05	2.66E+05	5.88E+04	9.96E+04	1.51E+05	3.20E+05	1.20E+05	4.95E+05	4.66E+05	3.82E+05	--	--
mws2623	2.81E+02	2.82E+02	C18H34O2	[M-H] ⁻	11-Octadecanoic acid(Vaccenic acid)	Lipids	Free fatty acids	506-17-2	A	3.55E+05	5.53E+05	6.96E+05	3.34E+05	4.26E+05	3.32E+05	5.62E+05	1.95E+06	4.89E+05	4.78E+05	7.93E+05	7.25E+05	--	--
mws0396	2.81E+02	2.82E+02	C18H34O2	[M-H] ⁻	Elaidic Acid	Lipids	Free fatty acids	112-79-8	A	1.07E+06	1.66E+06	1.93E+06	1.01E+06	1.34E+06	9.29E+05	1.62E+06	5.87E+06	1.47E+06	1.61E+06	2.41E+06	2.31E+06	--	--
pme1178	2.84E+02	2.83E+02	C10H13N5O5	[M+H] ⁺	Guanosine	Nucleotides and derivatives	Nucleotides and derivatives	118-00-3	A	5.86E+05	7.64E+05	1.34E+06	4.40E+05	5.47E+05	7.23E+05	6.69E+05	6.64E+05	7.57E+05	7.39E+05	8.19E+05	7.57E+05	C00387	ko00230,ko01100,ko02010
mws0668	2.83E+02	2.84E+02	C10H12N4O6	[M-H] ⁻	Xanthosine	Nucleotides and derivatives	Nucleotides and derivatives	146-80-5	B	3.52E+05	4.28E+05	5.13E+05	9.65E+04	2.14E+05	1.99E+05	7.60E+04	1.08E+05	1.44E+05	2.27E+05	2.37E+05	1.93E+05	C01762	ko00230,ko00232,ko01100,ko01110,ko02010
mws1489	2.83E+02	2.84E+02	C18H36O2	[M-H] ⁻	Stearic Acid	Lipids	Free fatty acids	57-11-4	A	2.24E+07	2.57E+07	2.32E+07	2.30E+07	2.18E+07	2.24E+07	2.56E+07	2.69E+07	2.52E+07	2.43E+07	2.54E+07	2.33E+07	--	--
pmm001511	2.85E+02	2.86E+02	C13H18O7	[M-H] ⁻	3-Hydroxy-5-Methylphenol-1-Oxy-β-D-Glucose	Phenolic acids	Phenolic acids	-	B	7.96E+03	2.24E+04	1.98E+04	1.22E+04	1.10E+04	1.08E+04	6.84E+03	8.77E+03	2.99E+04	1.37E+04	1.58E+04	1.55E+04	--	--

pmb3081	2.89E+02	2.90E+02	C6H11PO11	[M-H]-	Glucarate O-Phosphoric acid	Others	Saccharides and Alcohols	-	B	7.07E+06	9.33E+06	8.78E+06	9.26E+06	7.69E+06	8.68E+06	8.62E+06	8.19E+06	6.68E+06	5.73E+06	8.25E+06	8.57E+06	--	--
pme0460	2.91E+02	2.90E+02	C15H14O6 C15H14O6	[M+H]+	L-Epicatechin	Flavonoids	Flavanols	490-46-0	A	1.92E+06	5.38E+06	3.13E+06	2.75E+06	3.04E+06	3.25E+06	1.26E+06	5.81E+06	4.56E+06	4.95E+06	3.92E+06	3.85E+06	C09727	ko00941,ko01100,ko01110
mws0054	2.89E+02	2.90E+02	6	[M-H]-	Catechin	Flavonoids	Flavanols	154-23-4	A	1.26E+06	4.63E+06	1.67E+06	2.57E+06	1.55E+06	1.28E+06	6.01E+05	2.35E+06	1.62E+06	2.62E+06	2.97E+06	2.10E+06	C06562	ko00941,ko01110
mws2120	2.91E+02	2.92E+02	C13H8O8 C18H30O	[M-H]-	Brevifolin carboxylic acid	Phenolic acids	Phenolic acids	18490-95-4	B	3.00E+04	6.38E+04	3.59E+04	3.27E+04	2.15E+04	3.27E+04	2.35E+04	6.27E+04	3.20E+04	3.89E+04	4.02E+04	2.55E+04	--	--
pmb2792	2.93E+02	2.94E+02	3	[M-H]-	13-HOTrE(r) 9S-Hydroxy-10E,12E-octadecadienoic acid	Lipids	Free fatty acids	74784-20-6	B	3.15E+04	2.87E+04	2.26E+04	2.46E+04	3.76E+04	2.62E+04	2.55E+04	2.60E+04	3.37E+04	3.75E+04	3.58E+04	3.63E+04	--	--
pmm001688	2.95E+02	2.96E+02	C18H32O3 C18H32O3	[M-H]-	12,13-EODE 9-Hydroxy-10,12-octadecadienoic acid	Lipids	Free fatty acids	-	A	2.70E+03	3.17E+03	6.26E+03	3.58E+03	4.59E+03	2.99E+03	4.85E+03	9.47E+03	4.84E+03	7.28E+03	6.46E+03	5.04E+03	--	--
pmb2799	2.95E+02	2.96E+02	3	[M-H]-	12,13-EODE 9-Hydroxy-10,12-octadecadienoic acid	Lipids	Free fatty acids	6799-85-5	A	1.58E+04	1.04E+04	5.02E+04	6.07E+03	4.67E+03	2.44E+03	1.36E+03	1.45E+04	4.51E+03	1.17E+04	1.05E+04	1.12E+04	--	--
Rfmb091	2.95E+02	2.96E+02	C18H32O3	[M-H]-	13-Hydroxy-9,11-octadecadienoic acid	Lipids	Free fatty acids	15514-85-9	A	3.70E+03	3.55E+03	4.76E+03	4.68E+03	3.84E+03	2.28E+03	3.63E+03	7.93E+03	4.60E+03	6.12E+03	5.20E+03	5.37E+03	--	--
Rfmb090	2.95E+02	2.96E+02	C18H32O3	[M-H]-	13-Hydroxy-9,11-octadecadienoic acid	Lipids	Free fatty acids	5204-88-6	A	2.90E+03	5.07E+03	5.86E+03	3.47E+03	4.03E+03	3.46E+03	5.86E+03	9.43E+03	4.64E+03	7.38E+03	6.22E+03	7.00E+03	--	--
pmb2778	2.95E+02	2.96E+02	C18H32O3	[M-H]-	9,10-EODE 5'-Deoxy-5'-(methylthio)adenosine	Lipids	Free fatty acids	65167-83-1	B	9.47E+03	9.89E+03	1.98E+04	6.85E+03	9.93E+03	6.37E+03	2.72E+04	2.59E+04	1.42E+04	1.80E+04	1.69E+04	1.71E+04	--	--
pme1474	2.98E+02	2.97E+02	C11H15N5O3S	[M+H]+	Hydroxyguanosine	Nucleotides and derivatives	Nucleotides and derivatives	2457-80-9	A	3.40E+06	4.32E+06	3.23E+06	3.87E+06	3.27E+06	4.46E+06	4.11E+06	4.93E+06	4.70E+06	3.65E+06	3.95E+06	4.86E+06	C00170	ko00270,ko00908,ko01100
mws0724	2.98E+02	2.99E+02	C10H13N5O6	[M-H]-	Salicylic acid O-glycoside	Nucleotides and derivatives	Nucleotides and derivatives	3868-31-3	B	6.94E+04	6.63E+04	8.27E+04	1.08E+05	6.00E+04	8.50E+04	1.07E+05	4.95E+04	1.06E+05	5.99E+04	8.67E+04	8.47E+04	--	--
Zmhn001926	2.99E+02	3.00E+02	C13H16O8	[M-H]-	Isosalicylic acid O-glycoside	Phenolic acids	Phenolic acids	-	A	5.91E+05	9.29E+05	4.36E+05	7.42E+05	7.15E+05	8.56E+05	9.97E+05	8.12E+05	7.00E+05	6.67E+05	8.14E+05	8.96E+05	--	--
Zmxn001997	2.99E+02	3.00E+02	C13H16O8	[M-H]-	Glucosyloxybenzoic acid	Phenolic acids	Phenolic acids	-	A	4.28E+05	2.57E+05	3.05E+05	5.08E+05	5.79E+05	4.60E+05	4.59E+05	6.85E+05	7.36E+05	5.96E+05	6.56E+05	6.57E+05	--	--
Hmtn001302	2.99E+02	3.00E+02	C13H16O8 C15H10O	[M-H]-	Morin	Phenolic acids	Phenolic acids	-	A	8.19E+05	1.04E+06	5.70E+05	7.28E+05	8.61E+05	4.99E+05	1.46E+06	1.33E+06	7.30E+05	9.08E+05	8.08E+05	8.07E+05	--	--
pme3514	3.01E+02	3.02E+02	C15H10O7	[M-H]-	Quercetin	Flavonoids	Flavonols	6472-38-4	B	9.86E+03	1.40E+04	1.10E+04	1.06E+04	1.51E+04	1.97E+04	8.04E+03	7.91E+03	1.02E+04	1.43E+04	1.53E+04	1.73E+04	C10105	--
pme2954	3.03E+02	3.02E+02	C15H10O7	[M+H]+	Tetrahydroxy-Coumaronochromone	Flavonoids	Flavonols	117-39-5	A	7.88E+03	5.51E+03	3.79E+03	1.13E+04	1.20E+04	9.02E+03	6.62E+03	4.12E+03	5.44E+03	1.00E+04	6.86E+03	8.41E+03	C00389	ko00941,ko00944,ko01100,ko01110
Hmyp002315	3.03E+02	3.02E+02	C15H10O7	[M+H]+	Taxifolin	Others	Others	-	A	1.70E+05	4.15E+04	9.00E+00	3.05E+04	7.37E+04	3.34E+04	1.51E+04	9.00E+00	2.76E+04	1.05E+05	6.45E+04	1.00E+05	--	--
mws0044	3.03E+02	3.04E+02	C15H12O7	[M-H]-	Epigallocatechin	Flavonoids	Dihydroflavono	480-18-2	A	1.28E+04	2.55E+04	3.99E+04	3.17E+04	1.56E+05	6.04E+04	1.44E+04	5.04E+04	2.50E+04	5.56E+04	4.43E+04	4.73E+04	C01617	ko00941,ko01100,ko01110
mws0042	3.05E+02	3.06E+02	C15H14O7	[M-H]-	Epigallocatechin	Flavonoids	Flavanols	970-74-1	A	3.61E+05	3.70E+05	1.54E+05	2.18E+05	1.58E+05	2.16E+05	1.55E+05	1.86E+05	1.69E+05	2.68E+05	3.99E+05	3.23E+05	C12136	ko00941,ko01110
GQ512003	3.07E+02	3.06E+02	C15H22O3N4	[M+H]+	Fer-aggmatine	Alkaloids	Phenolamine	-	B	3.91E+04	4.11E+04	2.28E+04	3.31E+04	2.60E+04	3.10E+04	1.62E+04	3.39E+04	1.44E+04	3.09E+04	3.16E+04	3.46E+04	--	--
pme1086	3.06E+02	3.07E+02	C10H17N3O6S	[M-H]-	Glutathione reduced form	Amino acids and derivatives	Amino acids and derivatives	70-18-8	A	8.55E+05	6.91E+05	4.65E+05	2.13E+05	3.77E+04	6.77E+04	3.94E+04	9.00E+00	9.00E+00	3.18E+05	3.23E+05	2.07E+05	C00051	ko00270,ko00480,ko01100,ko02010
pmm001606	3.09E+02	3.10E+02	C20H38O2	[M-H]-	Eicosenoic acid	Lipids	Free fatty acids	26764-41-0	B	2.04E+04	4.28E+04	6.50E+04	2.21E+04	2.90E+04	2.03E+04	4.63E+04	6.59E+04	2.93E+04	5.45E+04	5.36E+04	5.76E+04	C16526	ko01040
pme3967	3.12E+02	3.11E+02	C12H17N5O5	[M+H]+	(Dimethylamino)guanosine	Nucleotides and derivatives	Nucleotides and derivatives	2140-67-2	B	5.16E+04	3.29E+04	2.77E+04	4.80E+04	3.62E+04	5.05E+04	3.50E+04	4.77E+04	5.63E+04	4.07E+04	5.16E+04	4.96E+04	--	--

Lmhn001477	3.11E+02	3.12E+02	C13H12O9	[M-H]-	Caffeoyltartaric acid(Caftaric acid)	Phenolic acids	Phenolic acids	67879-58-7	B	9.40E+04	1.07E+05	1.10E+05	3.36E+04	1.21E+05	1.25E+05	3.69E+04	4.30E+05	1.86E+05	1.88E+05	1.23E+05	1.51E+05	--	--
pmb2871	3.15E+02	3.16E+02	C13H16O9	[M-H]-	2,5-Dihydroxy benzoic acid O-hexside	Phenolic acids	Phenolic acids	-	A	4.90E+06	2.52E+06	2.48E+06	3.07E+06	3.43E+06	2.07E+06	2.50E+06	2.78E+06	2.71E+06	3.07E+06	3.37E+06	3.11E+06	--	--
pmm001367	3.15E+02	3.16E+02	C13H16O9	[M-H]-	acid-4-glucoside	Phenolic acids	Phenolic acids	-	A	4.44E+06	2.70E+06	2.31E+06	3.14E+06	3.14E+06	1.92E+06	2.75E+06	3.11E+06	2.45E+06	3.09E+06	3.34E+06	3.23E+06	--	--
Hmtn001120	3.15E+02	3.16E+02	C14H20O8	[M-H]-	5-(2-Hydroxyethyl)-2-O-glucosylohenol	Phenolic acids	Phenolic acids	-	A	9.95E+06	2.40E+06	2.72E+06	8.04E+05	2.78E+06	5.11E+05	1.13E+06	8.65E+05	1.26E+06	2.67E+06	2.34E+06	2.54E+06	--	--
pme3459	3.17E+02	3.16E+02	C20H28O3	[M+H]+	Caffeyl alcohol	Phenolic acids	Phenolic acids	469-83-0	B	1.23E+04	1.17E+04	1.27E+04	1.23E+04	1.17E+04	1.27E+04	1.57E+04	1.42E+04	1.49E+04	1.30E+04	1.27E+04	1.35E+04	C09066	--
YC512119	3.18E+02	3.17E+02	C18H39NO3	[M+H]+	Phytosphingosine	Others	Others	554-62-1	A	2.91E+04	2.78E+04	3.19E+04	2.43E+04	1.74E+04	1.94E+04	3.36E+04	1.96E+04	2.77E+04	2.63E+04	2.48E+04	2.63E+04	--	--
pmp001267	3.20E+02	3.19E+02	C21H37NO	[M+H]+	2-(Dodecylamino)-3-phenyl-1-propanol	Others	Others	-	B	9.87E+03	1.18E+04	1.14E+04	8.18E+03	6.34E+03	7.64E+03	1.16E+04	9.36E+03	9.91E+03	8.36E+03	8.59E+03	8.41E+03	--	--
mws0582	3.22E+02	3.21E+02	C11H19NS	[M+H]+	(methyl)glutathione	Amino acids and derivatives	Amino acids and derivatives	2922-56-7	B	3.86E+05	3.98E+05	3.04E+05	2.10E+05	3.52E+05	2.58E+05	3.20E+05	2.18E+05	1.58E+05	3.44E+05	3.43E+05	3.16E+05	C11347	--
pme3188	3.23E+02	3.24E+02	C9H13N2O9P	[M-H]-	Uridine 5'-monophosphate	Nucleotides and derivatives	Nucleotides and derivatives	58-97-9	A	2.33E+04	3.36E+04	6.35E+04	1.78E+04	2.02E+04	1.44E+04	4.87E+04	4.69E+04	5.35E+04	4.01E+04	5.24E+04	3.76E+04	C00105	ko00240,ko01100
Lmhn002140	3.25E+02	3.26E+02	C14H14O9	[M-H]-	Feruloyltartaric acid(Fertaric acid)	Phenolic acids	Phenolic acids	-	A	3.20E+06	1.69E+06	1.69E+06	1.81E+06	2.25E+06	1.72E+06	2.04E+06	2.76E+06	1.95E+06	2.05E+06	2.21E+06	2.28E+06	--	--
pmm001419	3.25E+02	3.26E+02	C15H18O8	[M-H]-	1-O-[(E)-p-Cumaroyl]-β-D-glucopyranose	Phenolic acids	Phenolic acids	-	A	5.71E+06	3.76E+06	4.88E+06	7.39E+06	8.74E+06	6.25E+06	6.73E+06	6.10E+06	8.11E+06	8.23E+06	7.54E+06	6.86E+06	--	--
Zmhn002301	3.25E+02	3.26E+02	C15H18O8	[M-H]-	p-Coumaric acid-O-glycoside	Phenolic acids	Phenolic acids	-	A	6.39E+05	1.76E+06	2.13E+06	1.72E+06	1.01E+06	8.33E+05	1.76E+06	8.81E+05	1.23E+06	1.34E+06	1.16E+06	1.17E+06	--	--
HmLn002835	3.25E+02	3.26E+02	C15H18O8	[M-H]-	Cis-p-coumaric acid 4-O-glycoside	Others	Others	-	A	2.41E+06	1.88E+06	2.32E+06	3.47E+06	3.24E+06	2.57E+06	3.36E+06	3.09E+06	4.86E+06	2.31E+06	2.96E+06	2.94E+06	--	--
pmm001690	3.27E+02	3.28E+02	C16H24O7	[M-H]-	3-Hydroxy-4-isopropylbenzyl alcohol 3-glucoside	Phenolic acids	Phenolic acids	-	B	3.26E+04	4.61E+04	4.43E+04	1.78E+04	1.87E+04	4.50E+04	6.20E+04	6.64E+04	2.70E+04	4.43E+04	4.84E+04	4.14E+04	--	--
HmLn002358	3.29E+02	3.30E+02	C14H18O9	[M-H]-	Vanillic acid-glucoside	Phenolic acids	Phenolic acids	-	B	5.72E+05	1.82E+05	1.90E+05	1.89E+05	5.71E+05	2.67E+05	1.81E+05	2.07E+05	2.20E+05	2.57E+05	2.30E+05	3.03E+05	--	--
Lmtn002565	3.29E+02	3.30E+02	C14H18O9	[M-H]-	1'-O-Vanilloyl-β-D-glucoside	Phenolic acids	Phenolic acids	-	A	5.68E+05	4.15E+05	3.52E+05	3.12E+05	3.89E+05	2.04E+05	2.22E+05	2.02E+05	2.51E+05	4.89E+05	3.99E+05	2.95E+05	--	--
Zmhn001375	3.29E+02	3.30E+02	C14H18O9	[M-H]-	Vanillic acid-C-glycoside	Others	Others	-	B	4.94E+04	9.21E+04	7.62E+04	1.01E+05	6.65E+04	1.27E+05	3.76E+04	6.38E+04	6.72E+04	1.08E+05	9.90E+04	7.45E+04	--	--
pmm001517	3.29E+02	3.30E+02	C15H22O8	[M-H]-	3,4,5-Trimethoxyphenyl-β-D-Glucopyranoside	Phenolic acids	Phenolic acids	-	B	1.22E+06	4.94E+05	9.55E+05	7.72E+05	6.87E+05	6.09E+05	3.91E+05	6.77E+05	8.68E+05	8.07E+05	7.50E+05	5.25E+05	--	--
pmm001694	3.29E+02	3.30E+02	C18H34O5	[M-H]-	9,10,13-Trihydroxy-11-octadecadienoic acid	Lipids	Free fatty acids	-	A	1.17E+04	8.08E+03	5.28E+04	5.93E+03	6.36E+03	4.32E+03	4.59E+04	4.09E+04	1.85E+04	2.68E+04	2.55E+04	2.42E+04	--	--

pnm001495	3.29E+02	3.30E+02	C19H38O4	[M-H]-	Hexadecanoic acid 2,3-dihydroxypropyl ester	Lipids	Glycerol ester	542-44-9	A	1.05E+04	7.43E+03	4.13E+04	4.77E+03	6.54E+03	4.29E+03	3.96E+04	3.75E+04	1.54E+04	1.93E+04	2.07E+04	1.75E+04	--	--
pme3184	3.32E+02	3.31E+02	C10H14N5O6P	[M+H]+	Deoxyadenosine-5'-monophosphate	Nucleotides and derivatives	Nucleotides and derivatives	653-63-4	B	9.02E+04	8.10E+04	1.06E+05	1.34E+05	1.10E+05	1.19E+05	2.05E+05	1.58E+05	1.10E+05	1.38E+05	1.27E+05	9.99E+04	C00360	ko00230,ko01100
pnm001627	3.31E+02	3.32E+02	C13H16O10	[M-H]-	Glucogallin D-	Phenolic acids	Phenolic acids	58511-73-2	A	9.91E+04	9.00E+00	1.46E+05	1.13E+05	1.35E+05	9.00E+00	9.00E+00	9.00E+00	1.50E+05	1.34E+05	1.63E+05	1.73E+05	--	--
pmp000260	3.33E+02	3.32E+02	C13H16O10	[M+H]+	D-glucopyranoside	Phenolic acids	Phenolic acids	-	B	1.53E+04	5.45E+04	1.64E+04	1.44E+04	1.80E+04	1.94E+04	1.88E+04	7.91E+04	6.69E+04	4.08E+04	3.25E+04	2.63E+04	--	--
pnm001518	3.31E+02	3.32E+02	C13H16O10	[M-H]-	1-O-Galloyl-β-D-glucose	Phenolic acids	Phenolic acids	-	A	3.46E+04	3.61E+04	3.19E+04	3.40E+04	4.17E+04	3.37E+04	3.50E+04	6.32E+04	3.24E+04	4.84E+04	5.06E+04	4.15E+04	--	--
HmLn000659	3.31E+02	3.32E+02	C13H16O10	[M-H]-	3-O-Galloyl-β-D-glucose	Tannins	Tannin	-	B	1.21E+05	1.84E+05	1.34E+05	8.22E+04	1.72E+05	6.91E+04	9.82E+04	2.24E+05	8.58E+04	1.42E+05	1.31E+05	1.37E+05	--	--
HmLn000873	3.31E+02	3.32E+02	C13H16O10	[M-H]-	2-O-Galloyl-β-D-glucose	Tannins	Tannin	-	B	9.56E+05	3.25E+06	9.39E+05	7.23E+05	7.58E+05	9.40E+05	1.11E+06	4.34E+06	3.72E+06	2.20E+06	1.90E+06	2.00E+06	--	--
mws0675	3.35E+02	3.34E+02	C11H15N2O8P	[M+H]+	β-Nicotinamide mononucleotide	Nucleotides and derivatives	Nucleotides and derivatives	1094-61-7	B	2.81E+04	6.22E+04	1.16E+05	3.02E+04	4.95E+04	6.40E+04	6.29E+04	6.83E+04	8.14E+04	5.56E+04	5.56E+04	3.66E+04	C00455	ko00760,ko01100
mws5039	3.41E+02	3.40E+02	C15H16O9	[M+H]+	Esculin Hydrate	Lignans and Coumarins	Coumarins	66778-17-4	B	6.92E+04	4.34E+04	2.65E+04	2.10E+04	3.55E+04	3.30E+04	3.80E+04	2.95E+04	3.29E+04	3.74E+04	3.77E+04	3.77E+04	--	--
pnm001420	3.41E+02	3.42E+02	C15H18O9	[M-H]-	1-O-[(E)-Caffeoyl]-β-D-glucopyranose	Phenolic acids	Phenolic acids	-	A	4.08E+05	3.17E+05	5.94E+05	5.34E+05	5.44E+05	3.29E+05	3.60E+05	5.02E+05	7.03E+05	5.39E+05	5.68E+05	7.76E+05	--	--
Zmhn002242	3.41E+02	3.42E+02	C15H18O9	[M-H]-	Caffeoyl glucose	Phenolic acids	Phenolic acids	14364-08-0	A	2.12E+04	6.05E+03	1.82E+04	2.42E+03	1.51E+04	1.00E+04	8.50E+03	1.23E+04	9.70E+03	1.70E+04	1.40E+04	8.78E+03	C10433	--
mws1333	3.41E+02	3.42E+02	C12H22O11	[M-H]-	Melibiose D-(+)-	Others	Saccharides and Alcohols	585-99-9	A	1.61E+06	2.36E+06	1.96E+06	1.77E+06	2.17E+06	1.56E+06	1.63E+06	2.39E+06	1.79E+06	2.18E+06	1.75E+06	2.53E+06	C05402	ko00052,ko01100,ko02010
mws0264	3.41E+02	3.42E+02	C12H22O11	[M-H]-	Trehalose Anhydrous	Others	Saccharides and Alcohols	99-20-7	A	2.10E+06	2.70E+06	2.46E+06	2.29E+06	2.28E+06	2.22E+06	2.73E+06	2.38E+06	2.58E+06	1.72E+06	2.52E+06	2.46E+06	--	--
pme0519	3.41E+02	3.42E+02	C12H22O11	[M-H]-	D-(+)-Sucrose	Others	Saccharides and Alcohols	57-50-1	A	5.42E+06	5.68E+06	4.98E+06	4.45E+06	5.54E+06	4.50E+06	4.10E+06	3.73E+06	5.86E+06	4.86E+06	3.98E+06	4.86E+06	--	--
mws1080	3.41E+02	3.42E+02	C12H22O11	[M-H]-	Galactinol	Others	Saccharides and Alcohols	3687-64-7	A	9.52E+06	1.09E+07	9.61E+06	8.48E+06	8.27E+06	6.92E+06	8.99E+06	9.54E+06	7.66E+06	7.05E+06	9.70E+06	8.87E+06	--	--
mws5038	3.41E+02	3.42E+02	C12H22O11	[M-H]-	Isomaltulose	Others	Saccharides and Alcohols	13718-94-0	A	4.81E+06	5.76E+06	4.99E+06	3.54E+06	4.36E+06	3.85E+06	4.38E+06	5.02E+06	4.95E+06	4.85E+06	6.08E+06	5.45E+06	--	--
mws0380	3.41E+02	3.42E+02	C12H22O11	[M-H]-	Lactose	Others	Saccharides and Alcohols	63-42-3	A	1.60E+06	1.72E+06	1.32E+06	1.31E+06	1.76E+06	1.24E+06	1.66E+06	1.55E+06	1.65E+06	1.39E+06	1.51E+06	1.55E+06	--	--
pmb0801	3.46E+02	3.45E+02	C14H19NO9	[M+H]+	acid O-hexoside	Others	Vitamin	-	B	1.13E+05	9.24E+04	8.04E+04	1.04E+05	9.89E+04	1.28E+05	1.32E+05	1.16E+05	1.09E+05	1.20E+05	1.16E+05	1.07E+05	--	--
pmb0981	3.48E+02	3.47E+02	C10H14N5O7P	[M+H]+	Adenosine 5'-monophosphate	Nucleotides and derivatives	Nucleotides and derivatives	61-19-8	B	5.50E+05	1.07E+06	1.39E+06	4.92E+05	4.74E+05	4.44E+05	1.19E+06	9.95E+05	1.14E+06	9.14E+05	8.54E+05	8.87E+05	C00020	ko00230,ko00908,ko01100,ko01110
pmb2444	3.53E+02	3.52E+02	C21H36O4	[M+H]+	MAG(18:3)iso mer1	Lipids	Glycerol ester	-	B	1.91E+05	1.74E+05	1.40E+05	9.41E+04	9.98E+04	1.00E+05	1.04E+05	1.20E+05	1.09E+05	1.39E+05	1.41E+05	1.33E+05	--	--
mws1077	3.55E+02	3.54E+02	C16H18O9	[M+H]+	Scopolin	Lignans and Coumarins	Coumarins	531-44-2	B	3.99E+04	2.32E+04	2.91E+04	4.98E+04	3.66E+04	4.38E+04	4.91E+04	4.36E+04	2.98E+04	3.02E+04	3.91E+04	3.59E+04	C01527	ko00940,ko01110
pmp001283	3.55E+02	3.54E+02	C21H38O4	[M+H]+	Glycerol linoleate	Lipids	Glycerol ester	26545-74-4	B	1.23E+04	5.35E+03	9.81E+03	3.45E+03	4.34E+03	3.92E+03	9.77E+03	4.24E+03	8.43E+03	8.15E+03	7.26E+03	6.25E+03	--	--
pmb0164	3.55E+02	3.54E+02	C21H38O4	[M+H]+	MAG(18:2)iso mer1	Lipids	Glycerol ester	-	B	7.72E+03	5.10E+03	7.95E+03	4.46E+03	3.27E+03	2.54E+03	7.06E+03	4.11E+03	8.74E+03	6.63E+03	6.05E+03	5.51E+03	--	--
pmb0890	3.55E+02	3.54E+02	C21H38O4	[M+H]+	MAG(18:2) Feruloyl	Lipids	Glycerol ester	-	B	1.22E+05	1.04E+05	9.81E+04	7.47E+04	7.69E+04	6.95E+04	7.13E+04	1.09E+05	9.00E+04	1.08E+05	1.08E+05	9.58E+04	--	--
Zmhn002422	3.55E+02	3.56E+02	C16H20O9	[M-H]-	glucose	Phenolic acids	Phenolic acids	-	A	1.37E+06	7.68E+05	5.04E+05	1.39E+06	9.69E+05	4.25E+05	8.66E+05	1.74E+06	5.66E+05	1.05E+06	8.76E+05	6.15E+05	C17759	--
pmb2363	3.57E+02	3.56E+02	C21H40O4	[M+H]+	MAG(18:1)iso mer1	Lipids	Glycerol ester	-	B	2.29E+04	6.63E+03	7.27E+03	7.34E+03	6.72E+03	4.42E+03	8.87E+03	6.32E+03	1.06E+04	9.20E+03	8.43E+03	8.28E+03	--	--

pmb3107	3.59E+02	3.60E+02	C15H20O10	[M-H]-	Syringic acid O-glucoside	Phenolic acids	Phenolic acids	-	B	1.44E+05	1.07E+05	1.50E+05	1.12E+05	8.59E+04	1.30E+05	1.29E+05	1.14E+05	1.18E+05	1.35E+05	1.19E+05	1.39E+05	--	--	
pmb0998	3.64E+02	3.63E+02	C10H14N5O8P	[M+H]+	Guanosine 5'-monophosphate	Nucleotides and derivatives	Nucleotides and derivatives	85-32-5	B	1.95E+04	2.51E+04	5.14E+04	2.01E+04	2.58E+04	2.46E+04	5.12E+04	3.50E+04	3.57E+04	3.90E+04	3.84E+04	2.87E+04	C00144	ko00230,ko01100	
mws5040	3.65E+02	3.64E+02	C12H21O11Na	[M+H]+	Turanose 3-Prenyl-4-O-β-D-glucopyranosyl	Others	Saccharides and Alcohols	547-25-1	B	1.53E+06	2.18E+06	2.37E+06	1.18E+06	2.11E+06	1.92E+06	2.38E+06	2.06E+06	2.13E+06	1.53E+06	1.68E+06	1.63E+06	--	--	
Lmhn003598	3.67E+02	3.68E+02	C18H24O8	[M-H]-	oxy-4-hydroxyl-benzoic acid	Phenolic acids	Phenolic acids	-	B	9.50E+03	2.05E+04	6.61E+03	1.68E+04	7.63E+03	1.08E+04	1.28E+04	1.77E+04	2.26E+04	1.53E+04	1.86E+04	1.77E+04	--	--	
mws0232	3.77E+02	3.76E+02	C17H20N4O6	[M+H]+	Riboflavin N6-Succinyl	Others	Vitamin	83-88-5	B	2.80E+03	8.25E+03	9.00E+00	6.13E+03	8.47E+03	4.09E+03	7.22E+03	1.59E+04	1.45E+04	6.60E+03	5.19E+03	1.04E+04	C00255	ko00740,ko01100,ko01110,ko02010	
pme3337	3.84E+02	3.83E+02	C14H17N5O8	[M+H]+	Adenosine 1-O-β-D-Glucopyranosyl	Nucleotides and derivatives	Nucleotides and derivatives	4542-23-8	A	3.11E+05	3.59E+05	3.10E+05	2.58E+05	2.53E+05	2.60E+05	2.97E+05	3.57E+05	3.92E+05	2.99E+05	3.76E+05	3.13E+05	--	--	
pmb2940	3.85E+02	3.86E+02	C17H22O10	[M-H]-	sinapate	Phenolic acids	Phenolic acids	78185-48-5	A	1.86E+05	6.74E+04	1.09E+05	9.25E+04	9.97E+04	1.23E+05	9.29E+04	8.08E+04	8.30E+04	9.17E+04	9.42E+04	5.89E+04	--	--	
Zmhn002513	3.85E+02	3.86E+02	C17H22O10	[M-H]-	Isosinapic acid-hexoside	Phenolic acids	Phenolic acids	-	B	4.10E+04	3.77E+04	4.17E+04	6.23E+04	5.15E+04	4.58E+04	8.51E+04	4.71E+04	5.14E+04	4.89E+04	8.20E+04	5.24E+04	--	--	
mws0043	4.03E+02	4.02E+02	C21H22O8	[M+H]+	Nobiletin	Flavonoids	Flavonoid	478-01-3	B	5.78E+03	7.43E+03	2.54E+04	9.23E+03	6.39E+03	4.24E+03	4.88E+03	1.63E+04	6.64E+03	9.40E+03	1.03E+04	1.11E+04	C10112	--	
pme3007	4.03E+02	4.04E+02	C9H14N2O12P2	[M-H]-	Uridine 5'-diphosphate	Nucleotides and derivatives	Nucleotides and derivatives	27821-45-0	A	2.09E+04	3.30E+04	3.11E+04	1.52E+04	1.55E+04	1.32E+04	2.10E+04	1.56E+04	2.75E+04	2.13E+04	2.32E+04	1.52E+04	C00015	ko00240,ko00908,ko01100	
pmn001394	4.05E+02	4.06E+02	C20H22O9	[M-H]-	Tetrahydroxy-stilbene-2-O-D-glucopyranoside	Others	Stilbene	-	A	1.16E+06	8.81E+05	8.63E+05	8.19E+05	1.71E+06	9.06E+05	1.09E+06	1.14E+06	9.10E+05	7.80E+05	8.47E+05	1.16E+06	--	--	
Zmhn101746	4.05E+02	4.06E+02	C20H22O9	[M-H]-	Tetrahydroxy-stilbene-O-glucoside	Others	Stilbene	-	A	1.93E+05	2.41E+06	3.33E+06	4.97E+05	2.01E+05	4.41E+05	4.26E+05	3.05E+05	1.54E+06	1.32E+06	1.10E+06	1.06E+06	--	--	
Zmhn001746	4.05E+02	4.06E+02	C20H22O9	[M-H]-	Piceatannol-O-glucoside	Others	Stilbene	-	A	2.64E+05	3.32E+06	4.40E+06	5.32E+05	1.86E+05	7.80E+05	2.77E+05	7.06E+05	2.55E+06	1.16E+06	1.30E+06	1.01E+06	--	--	
Lmbp003668	4.19E+02	4.18E+02	C20H18O10	[M+H]+	Kaempferol-3-arabinopyranoside	Flavonoids	Flavonols	-	A	2.00E+05	1.55E+04	2.32E+04	9.00E+00	1.09E+05	9.00E+00	9.00E+00	9.00E+00	9.00E+00	9.00E+00	4.40E+04	3.70E+04	4.79E+04	--	--
mws2523	4.21E+02	4.22E+02	C12H23O14P	[M-H]-	Trehalose 6-phosphate	Others	Saccharides and Alcohols	4484-88-2	B	1.36E+05	1.29E+05	2.09E+05	1.45E+05	8.40E+04	6.34E+04	1.16E+05	1.07E+05	9.58E+04	1.30E+05	1.46E+05	1.27E+05	C00689	ko00500,ko01100	
Hmcp005535	4.25E+02	4.24E+02	C30H48O19H40N	[M+H]+	α-Amyrenone	Terpenoids	Triterpene	638-96-0	A	3.59E+04	3.01E+04	2.44E+04	2.90E+04	3.39E+04	2.78E+04	3.30E+04	2.70E+04	3.96E+04	2.81E+04	2.94E+04	2.69E+04	--	--	
pmb0864	4.26E+02	4.25E+02	C19H40N7O7P	[M+H]+	LysoPE 14:0	Lipids	LPE	-	B	9.38E+03	1.94E+04	4.20E+04	1.32E+04	9.92E+03	1.31E+04	2.55E+04	3.18E+04	2.44E+04	2.30E+04	2.25E+04	2.19E+04	--	--	
pme0321	4.31E+02	4.32E+02	C21H20O10	[M-H]-	Kaempferol 7-O-rhamnoside	Flavonoids	Flavonols	20196-89-8	B	1.85E+05	7.10E+03	2.68E+03	3.99E+03	2.36E+04	4.72E+03	1.56E+03	2.63E+03	4.61E+03	3.57E+04	2.48E+04	3.19E+04	--	--	
mws0072	4.33E+02	4.32E+02	C21H20O10	[M+H]+	Apigenin 5-O-glucoside	Flavonoids	Flavonoid	28757-27-9	B	2.12E+04	1.07E+05	1.28E+05	3.38E+04	1.31E+04	1.42E+04	9.30E+03	1.26E+04	2.87E+04	3.68E+04	4.31E+04	4.23E+04	--	--	
mws0048	4.31E+02	4.32E+02	C21H20O10	[M-H]-	Vitexin	Flavonoids	Flavonoid carbonoside	3681-93-4	B	4.81E+03	1.48E+04	5.69E+03	7.66E+03	6.27E+03	1.34E+04	4.31E+03	1.59E+04	1.68E+04	1.34E+04	1.96E+04	1.15E+04	C01460	ko00941,ko00944	
Lmbp003737	4.33E+02	4.32E+02	C21H20O10	[M+H]+	Kaempferol-3-O-rhamnoside	Flavonoids	Flavonols	482-39-3	A	3.34E+05	1.14E+04	4.56E+03	5.93E+03	4.38E+04	7.47E+03	1.75E+03	4.30E+03	6.05E+03	5.09E+04	4.79E+04	6.19E+04	C16911	ko00944	
Lmdp003577	4.33E+02	4.32E+02	C21H20O10	[M+H]+	Genistin(Genistein 7-O-Glucoside)	Flavonoids	Isoflavones	-	B	2.89E+04	1.39E+04	2.45E+04	1.73E+04	1.91E+04	1.82E+04	1.90E+04	2.48E+04	2.23E+04	3.37E+04	2.73E+04	2.62E+04	C09126	ko00943	
pme3392	4.33E+02	4.33E+02	C21H21O10+	[M]+	Pelargonidin 3-O-glucoside	Flavonoids	Anthocyanins	47684-27-5	B	8.89E+05	1.06E+06	1.41E+06	6.13E+05	7.02E+05	6.90E+05	3.25E+05	4.10E+05	6.59E+05	7.73E+05	7.90E+05	7.30E+05	C12137	ko00942,ko01100,ko01110	

mws4183	4.33E+02	4.34E+02	C20H18O11	[M-H]-	Quercetin-3-O- α -L-arabinopyranoside (guajaverin)	Flavonoids	Flavonols	22255-13-6	A	3.05E+05	7.74E+04	1.06E+05	2.27E+04	1.95E+05	3.00E+04	2.86E+04	2.13E+04	3.14E+04	1.16E+05	9.72E+04	9.41E+04	--	--
mws2186	4.35E+02	4.34E+02	C20H18O11	[M+H]+	Avicularin	Flavonoids	Flavonols	572-30-5	A	7.67E+05	1.47E+05	2.35E+05	7.32E+04	5.44E+05	8.56E+04	8.80E+04	7.87E+04	7.11E+04	2.63E+05	3.01E+05	2.68E+05	--	--
Lmdp003509	4.35E+02	4.34E+02	C20H18O11	[M+H]+	Quercetin 3-O- β -D-xylopyranoside	Flavonoids	Flavonols	549-32-6	B	7.91E+05	1.70E+05	2.33E+05	7.00E+04	5.43E+05	9.14E+04	8.59E+04	9.31E+04	8.29E+04	1.86E+05	2.88E+05	2.53E+05	--	--
mws1360	4.33E+02	4.34E+02	C21H22O10	[M-H]-	Engeletin	Flavonoids	Dihydroflavono	572-31-6	A	1.20E+06	2.76E+05	1.65E+05	2.03E+05	5.91E+05	1.52E+05	2.42E+05	2.07E+05	1.49E+05	3.78E+05	4.07E+05	5.34E+05	--	--
mws1179	4.33E+02	4.34E+02	C21H22O10	[M-H]-	Naringenin-7-O-glucoside	Flavonoids	Dihydroflavone	529-55-5	A	1.61E+05	1.08E+05	1.26E+05	8.69E+04	1.74E+05	1.39E+05	1.90E+05	1.63E+05	1.24E+05	1.48E+05	1.23E+05	1.15E+05	--	--
Zmhn003534	4.33E+02	4.34E+02	C21H22O10	[M-H]-	Naringenin-O-glucoside	Flavonoids	Flavonoid	-	A	1.21E+05	1.26E+05	1.35E+05	9.21E+04	1.69E+05	9.34E+04	8.78E+04	1.62E+05	1.04E+05	1.12E+05	1.64E+05	1.20E+05	--	--
mws2118	4.35E+02	4.36E+02	C21H24O10	[M-H]-	Phloretin 2'-O-glucoside	Flavonoids	Isoflavones	60-81-1	A	1.80E+05	1.50E+05	1.40E+05	8.26E+04	1.38E+05	9.87E+04	6.24E+04	1.62E+05	7.99E+04	1.17E+05	1.30E+05	1.84E+05	--	--
mws1397	4.41E+02	4.42E+02	C22H18O10	[M-H]-	(-)-Epicatechin gallate	Flavonoids	Flavanols	1257-08-5	A	3.09E+04	2.69E+05	1.10E+05	3.31E+04	3.84E+04	6.73E+04	1.51E+04	1.69E+05	9.64E+05	3.06E+05	2.77E+05	2.65E+05	--	--
mws0355	4.41E+02	4.42E+02	C22H18O10	[M-H]-	(-)-Catechin gallate	Flavonoids	Flavanols	130405-40-2	A	4.05E+04	2.52E+05	1.15E+05	3.30E+04	3.77E+04	1.01E+05	2.57E+04	1.79E+05	1.08E+06	2.85E+05	1.99E+05	2.80E+05	--	--
mws0045	4.49E+02	4.48E+02	C21H20O11	[M+H]+	Quercitrin	Flavonoids	Flavonols	522-12-3	A	1.04E+06	2.31E+05	8.31E+04	1.73E+05	4.59E+05	1.60E+05	1.84E+05	1.89E+05	1.09E+05	3.60E+05	3.85E+05	3.35E+05	--	--
mws0089	4.47E+02	4.48E+02	C21H20O11	[M-H]-	Kaempferol 7-O-glucoside	Flavonoids	Flavonols	16290-07-6	A	2.53E+06	3.97E+05	5.95E+05	4.29E+04	1.53E+06	4.12E+04	2.45E+04	6.60E+04	5.46E+04	6.68E+05	6.49E+05	7.49E+05	--	--
pmb3024	4.47E+02	4.48E+02	C21H20O11	[M-H]-	Luteolin C-hexoside	Flavonoids	Flavonoid	-	B	1.44E+04	1.97E+04	1.05E+04	1.54E+04	1.25E+04	6.21E+03	2.88E+03	2.38E+04	1.49E+04	1.49E+04	2.00E+04	9.61E+03	--	--
mws2209	4.47E+02	4.48E+02	C21H20O11	[M-H]-	Astragalin (Kaempferol 3-O-Glucoside)	Flavonoids	Flavonols	480-10-4	A	2.14E+06	3.65E+05	5.39E+05	5.86E+04	1.47E+06	5.38E+04	3.87E+04	4.73E+04	4.87E+04	5.17E+05	6.73E+05	7.42E+05	--	--
pnm001405	4.47E+02	4.48E+02	C21H20O11	[M-H]-	Luteolin-7-O-glucoside	Flavonoids	Flavonoid	5373-11-5	A	8.02E+06	1.84E+06	3.10E+06	1.53E+06	4.74E+06	1.25E+06	1.63E+06	1.86E+06	2.02E+06	2.49E+06	3.14E+06	3.25E+06	C03951	ko00944
mws0913	4.47E+02	4.48E+02	C21H20O11	[M-H]-	Trifolin	Flavonoids	Flavonols	23627-87-4	A	5.27E+05	7.64E+04	1.16E+05	2.35E+04	3.26E+05	1.17E+04	8.59E+03	3.02E+04	2.23E+04	2.35E+05	9.73E+04	1.33E+05	C12626	ko00944
Hmpp003270	4.49E+02	4.48E+02	C21H20O11	[M+H]+	Luteolin-4'-O- β -D-glucoside	Flavonoids	Flavonoid	-	A	1.46E+07	1.69E+06	3.23E+06	3.27E+05	8.73E+06	3.17E+05	1.76E+05	3.22E+05	3.10E+05	4.47E+06	3.84E+06	3.43E+06	--	--
Hmpp003391	4.49E+02	4.48E+02	C21H20O11	[M+H]+	Luteolin-3'-O- β -D-glucoside	Flavonoids	Flavonoid	-	A	1.43E+07	1.75E+06	3.24E+06	3.59E+05	9.12E+06	3.66E+05	1.96E+05	2.96E+05	3.33E+05	3.77E+06	3.86E+06	4.22E+06	--	--
Lmbp003393	4.49E+02	4.48E+02	C21H20O11	[M+H]+	Quercetin-3-O- α -L-rhamnopyranoside	Flavonoids	Flavonols	-	A	1.25E+07	1.62E+06	2.96E+06	3.40E+05	8.52E+06	3.35E+05	1.92E+05	2.85E+05	2.84E+05	3.96E+06	4.52E+06	3.98E+06	--	--
Hmcp002316	4.49E+02	4.48E+02	C21H20O11	[M+H]+	Isorhamnetin-O-Pentoside	Flavonoids	Flavonols	-	B	5.10E+04	2.02E+04	4.00E+04	1.40E+04	2.93E+04	8.38E+03	7.55E+03	1.05E+04	1.21E+04	2.32E+04	2.25E+04	1.85E+04	--	--
Zmhn003410	4.47E+02	4.48E+02	C21H20O11	[M-H]-	Orientin	Flavonoids	Flavonoid carbonoside	28608-75-5	A	3.09E+06	2.33E+05	6.06E+05	3.78E+04	1.49E+06	3.82E+04	3.70E+04	4.66E+04	5.39E+04	5.71E+05	6.50E+05	5.31E+05	C10114	--
Lmmp003422	4.49E+02	4.48E+02	C21H20O11	[M+H]+	O- β -d-glucopyranoside	Flavonoids	Flavonols	-	A	1.11E+07	1.78E+06	3.36E+06	3.32E+05	8.51E+06	3.87E+05	1.95E+05	2.71E+05	3.07E+05	4.05E+06	4.52E+06	4.09E+06	--	--
pmb0550	4.49E+02	4.49E+02	C21H21O11+	[M]+	Cyanidin 3-O-glucoside (Kuromanin)	Flavonoids	Anthocyanins	47705-70-4	A	7.29E+07	8.01E+07	9.19E+07	5.13E+07	6.50E+07	5.30E+07	3.32E+07	3.41E+07	3.55E+07	5.62E+07	6.08E+07	5.59E+07	C08604	ko00942
pml0027	4.49E+02	4.49E+02	C21H21O11+	[M]+	Cyanidin 3-O-galactoside	Flavonoids	Anthocyanins	142506-26-1	B	8.04E+07	8.19E+07	1.00E+08	5.88E+07	7.14E+07	5.35E+07	3.95E+07	4.00E+07	4.07E+07	7.16E+07	5.78E+07	6.64E+07	C08647	--
pmb3023	4.49E+02	4.50E+02	C21H22O11	[M-H]-	Eriodictyol C-hexoside	Flavonoids	Dihydroflavone	-	B	2.75E+05	8.86E+05	4.33E+05	1.99E+05	2.00E+05	1.47E+05	1.22E+05	2.09E+05	2.30E+05	3.27E+05	3.44E+05	3.24E+05	--	--

pnn001416	4.51E+02	4.52E+02	C24H2009	[M-H]-	Catechin-(7,8-bc)-4a-(3,4-dihydroxyphenyl)-dihydro-2-(3H)-pyranone	Flavonoids	Flavanols	-	A	8.28E+05	6.47E+05	2.95E+05	3.44E+05	5.27E+05	4.21E+05	2.29E+05	3.17E+05	4.33E+05	4.66E+05	5.63E+05	5.02E+05	--	--
pnn001415	4.51E+02	4.52E+02	C24H2009	[M-H]-	Catechin-(7,8-bc)-4β-(3,4-dihydroxyphenyl)-dihydro-2-(3H)-pyranone	Flavonoids	Flavanols	-	A	2.05E+04	3.40E+04	1.42E+04	2.37E+04	1.79E+04	2.05E+04	2.16E+04	2.92E+04	2.86E+04	2.90E+04	2.79E+04	1.56E+04	--	--
pmb0876	4.54E+02	4.53E+02	C21H44N07P	[M+H]+	LysoPE 16:0	Lipids	LPE	53862-35-4	A	3.70E+05	1.54E+06	3.21E+06	1.18E+06	5.89E+05	7.94E+05	1.76E+06	2.29E+06	1.54E+06	1.48E+06	1.63E+06	1.53E+06	--	--
pmd0160	4.52E+02	4.53E+02	C21H44N07P	[M-H]-	LysoPE 16:0(2n isomer)	Lipids	LPE	-	A	3.29E+05	1.43E+06	2.84E+06	1.04E+06	5.64E+05	7.68E+05	1.49E+06	1.99E+06	1.41E+06	1.43E+06	1.32E+06	1.36E+06	--	--
mws1420	4.55E+02	4.54E+02	C28H22O6	[M+H]+	ε-Viniferin	Others	Stilbene	62218-08-0	A	1.89E+04	2.57E+05	4.40E+05	8.68E+04	6.80E+04	6.98E+04	1.46E+05	5.60E+04	5.11E+05	3.15E+05	2.93E+05	2.88E+05	C10289	--
pmp001093	4.55E+02	4.54E+02	C26H30O7	[M+H]+	Dihydroobacunone	Others	Others	-	B	6.05E+04	5.27E+04	5.35E+04	6.24E+04	8.01E+04	6.51E+04	5.96E+04	6.93E+04	7.16E+04	6.64E+04	7.20E+04	6.38E+04	--	--
pnn001700	4.55E+02	4.56E+02	C30H48O3	[M-H]-	24,30-Dihydroxy-12(13)-enolupinol	Terpenoids	Triterpene	-	A	8.66E+06	8.35E+06	7.85E+06	9.69E+06	1.15E+07	8.78E+06	1.11E+07	1.04E+07	8.06E+06	9.03E+06	1.11E+07	9.90E+06	--	--
mws1389	4.55E+02	4.56E+02	C30H48O3	[M-H]-	Oleanolic acid	Terpenoids	Triterpene	508-02-1	A	4.06E+03	3.94E+03	3.67E+03	4.25E+03	4.75E+03	3.78E+03	4.61E+03	4.12E+03	3.18E+03	4.28E+03	4.89E+03	4.89E+03	--	--
mws0351	4.57E+02	4.58E+02	C22H18O11	[M-H]-	Gallate catechin gallate	Flavonoids	Flavanols	4233-96-9	B	1.10E+04	2.59E+04	1.34E+04	9.11E+03	9.09E+03	1.14E+05	9.00E+00	9.00E+00	9.00E+00	4.60E+04	4.54E+04	3.06E+04	--	--
mws2220	4.57E+02	4.58E+02	C22H18O11	[M-H]-	Gallocatechin 3-O-gallate	Flavonoids	Flavanols	5127-64-0	B	8.16E+03	2.83E+04	2.28E+04	2.79E+04	7.18E+03	2.15E+05	8.15E+03	7.65E+03	5.78E+03	4.69E+04	4.35E+04	3.60E+04	--	--
mws4167	4.63E+02	4.62E+02	C21H18O12	[M+H]+	Luteolin 7-O-glucuronide	Flavonoids	Flavonoid	29741-10-4	B	3.21E+06	3.47E+05	3.53E+05	1.80E+05	7.87E+05	2.00E+05	2.61E+05	4.45E+05	3.37E+05	6.45E+05	7.82E+05	6.68E+05	--	--
pnn001702	4.61E+02	4.62E+02	C21H18O12	[M-H]-	Tetrahydroxy-flavone-7-O-β-D-glucuronide	Flavonoids	Flavonoid	-	A	3.51E+04	2.13E+04	1.10E+04	9.00E+00	4.14E+04	8.23E+03	6.01E+03	7.66E+03	1.09E+04	1.26E+04	2.23E+04	2.61E+04	--	--
Lmzn001894	4.61E+02	4.62E+02	C21H18O12	[M-H]-	Kaempferol-3-O-β-D-glucuronide	Flavonoids	Flavonols	-	A	4.07E+04	1.14E+04	1.86E+04	8.20E+03	3.48E+04	1.31E+04	4.36E+03	7.63E+03	2.45E+03	3.38E+04	1.31E+04	2.12E+04	--	--
pmp000579	4.63E+02	4.62E+02	C22H22O11	[M+H]+	Diosmetin-7-O-galactoside	Flavonoids	Flavonoid	-	B	6.58E+04	7.08E+04	6.77E+04	8.34E+04	1.15E+05	6.48E+04	4.39E+04	9.93E+04	7.57E+04	1.01E+05	9.63E+04	1.04E+05	--	--
pmb2999	4.61E+02	4.62E+02	C22H22O11	[M-H]-	Chrysoeriol 5-O-hexoside	Flavonoids	Flavonoid	-	A	5.94E+06	2.10E+06	3.13E+06	1.15E+06	4.88E+06	1.40E+06	1.03E+06	1.04E+06	1.12E+06	2.78E+06	2.75E+06	1.83E+06	--	--
Zmhn003191	4.61E+02	4.62E+02	C22H22O11	[M-H]-	O-hexoside	Flavonoids	Flavonoid	20013-23-4	B	1.87E+05	6.44E+04	1.03E+05	3.46E+04	1.54E+05	3.79E+04	3.58E+04	4.17E+04	4.19E+04	1.07E+05	8.55E+04	1.11E+05	C05990	--
mws2210	4.63E+02	4.63E+02	C22H23O11+	[M]+	Isoscoparin Peonidin 3-O-glucoside	Flavonoids	Anthocyanins	6906-39-4	B	1.42E+06	1.90E+06	3.97E+06	1.28E+06	1.58E+06	1.54E+06	7.75E+05	1.15E+06	1.71E+06	1.88E+06	1.72E+06	1.74E+06	--	--
pma1590	4.63E+02	4.63E+02	C22H23O11+	[M]+	Peonidin O-hexoside	Flavonoids	Anthocyanins	-	B	1.30E+06	1.61E+06	3.26E+06	1.18E+06	1.52E+06	1.38E+06	6.96E+05	9.73E+05	1.42E+06	1.72E+06	1.66E+06	1.51E+06	--	--
mws0856	4.63E+02	4.64E+02	C21H20O12	[M-H]-	Spiraeoside	Flavonoids	Flavonols	20229-56-5	B	2.17E+07	1.04E+07	1.33E+07	5.38E+06	2.02E+07	6.19E+06	4.29E+06	5.32E+06	5.15E+06	1.24E+07	1.10E+07	1.25E+07	--	--
pme3211	4.63E+02	4.64E+02	C21H20O12	[M-H]-	Quercetin 3-O-glucoside(Isotrifoliin)	Flavonoids	Flavonols	21637-25-2	A	2.81E+07	9.93E+06	1.56E+07	5.72E+06	2.14E+07	6.97E+06	4.02E+06	5.99E+06	5.90E+06	1.36E+07	1.22E+07	1.39E+07	C05623	ko00944,ko01100,ko01110
pmp001309	4.65E+02	4.64E+02	C21H20O12	[M+H]+	Hydroxykaempferol-7-O-glucoside	Flavonoids	Flavonols	-	A	3.35E+06	1.28E+06	1.72E+06	8.21E+05	2.46E+06	7.77E+05	5.95E+05	7.62E+05	5.86E+05	1.32E+06	1.42E+06	1.96E+06	--	--
pmp000580	4.65E+02	4.64E+02	C21H20O12	[M+H]+	Isoquercitrin(Quercetin 3-O-β-D-glucoside)	Flavonoids	Flavonols	482-35-9	A	3.61E+07	2.07E+07	2.88E+07	1.12E+07	3.75E+07	1.36E+07	7.73E+06	1.35E+07	1.04E+07	2.67E+07	2.59E+07	2.61E+07	--	--

mws0061	4.63E+02	4.64E+02	C21H20012	[M-H]-	Hyperin	Flavonoids	Flavonols	482-36-0	A	3.38E+07	1.42E+07	2.06E+07	9.52E+06	2.84E+07	1.00E+07	1.11E+07	7.98E+06	7.68E+06	1.84E+07	2.21E+07	2.14E+07	--	--
Hmcn001884	4.63E+02	4.64E+02	C21H20012	[M-H]-	Hydroxyluteolin 5-glucoside	Flavonoids	Flavonoid	-	B	1.02E+07	3.91E+06	5.22E+06	1.63E+06	7.96E+06	2.95E+06	2.13E+06	1.72E+06	1.21E+06	4.46E+06	3.42E+06	4.18E+06	--	--
mws1329	4.63E+02	4.64E+02	C21H20012	[M-H]-	Quercetin-7-O-Glucoside	Flavonoids	Flavonols	491-50-9	A	2.13E+07	8.71E+06	1.18E+07	4.56E+06	2.12E+07	5.64E+06	3.88E+06	4.88E+06	3.42E+06	7.88E+06	9.23E+06	1.10E+07	--	--
Lmdp003286	4.65E+02	4.64E+02	C21H20012	[M+H]+	Isohyperoside	Flavonoids	Flavonols	35589-21-0	A	4.17E+06	1.10E+06	1.64E+06	6.71E+05	2.73E+06	7.83E+05	6.60E+05	6.56E+05	6.92E+05	2.04E+06	1.25E+06	1.74E+06	--	--
pme1598	4.63E+02	4.64E+02	C22H24011	[M-H]-	Hesperetin 5-O-glucoside	Flavonoids	Dihydroflavono	69651-80-5	A	2.40E+07	8.41E+06	1.30E+07	5.50E+06	1.83E+07	4.78E+06	3.97E+06	5.92E+06	5.52E+06	1.11E+07	1.05E+07	1.30E+07	--	--
pmb2957	4.65E+02	4.67E+02	C24H19010+	[M-2H]-	Cyanidin O-syringic acid	Flavonoids	Anthocyanins	-	A	6.83E+06	6.28E+06	8.75E+06	4.95E+06	5.61E+06	3.91E+06	2.44E+06	2.67E+06	2.78E+06	6.55E+06	7.07E+06	5.04E+06	--	--
pmd0130	4.68E+02	4.67E+02	C22H46N07P	[M+H]+	LysoPC 14:0(2n isomer)	Lipids	LPC	-	B	3.39E+04	5.10E+04	9.46E+04	4.00E+04	3.67E+04	3.82E+04	8.99E+04	9.50E+04	8.15E+04	6.07E+04	5.96E+04	6.49E+04	--	--
pmm001704	4.69E+02	4.70E+02	C30H4604	[M-H]-	2,3-Dihydroxy 5(6),12(13)dien	Terpenoids	Triterpene	-	A	1.45E+05	1.01E+05	7.73E+04	9.32E+04	1.31E+05	8.12E+04	8.79E+04	7.74E+04	8.10E+04	1.06E+05	1.03E+05	1.04E+05	--	--
Hmjn008136	4.69E+02	4.70E+02	C30H4604	[M-H]-	Camaldulenic acid	Terpenoids	Triterpene	71850-15-2	A	2.11E+06	1.43E+06	1.09E+06	1.18E+06	2.04E+06	1.04E+06	1.18E+06	1.04E+06	1.07E+06	1.58E+06	1.44E+06	1.40E+06	--	--
pmm001705	4.71E+02	4.72E+02	C30H4804	[M-H]-	3,24-Dihydroxy-17,21-semiacetal-12(13)oleanolic fruit	Terpenoids	Triterpene	-	B	2.87E+05	2.26E+05	2.10E+05	2.49E+05	3.17E+05	1.94E+05	3.11E+05	2.66E+05	2.40E+05	2.62E+05	3.00E+05	2.65E+05	--	--
pmm001706	4.71E+02	4.72E+02	C30H4804	[M-H]-	Hydroxyoleanolic acid	Terpenoids	Triterpene	26707-60-8	A	2.87E+05	1.96E+05	1.87E+05	2.21E+05	3.08E+05	1.90E+05	2.59E+05	2.06E+05	1.93E+05	2.57E+05	2.46E+05	2.25E+05	--	--
mws1610	4.71E+02	4.72E+02	C30H4804	[M-H]-	Maslinic acid	Terpenoids	Triterpene	4373-41-5	B	5.48E+05	3.70E+05	3.51E+05	3.81E+05	5.48E+05	3.25E+05	4.03E+05	3.52E+05	3.34E+05	4.61E+05	4.07E+05	4.13E+05	C16939	--
pmm001641	4.75E+02	4.76E+02	C22H20012	[M-H]-	Kaempferide 3-O-β-D-glucuronide	Flavonoids	Flavonols	-	B	1.78E+04	3.30E+03	5.81E+03	9.00E+00	1.02E+04	9.00E+00	9.00E+00	5.72E+03	9.00E+00	5.81E+03	8.73E+03	1.31E+04	--	--
pmb0874	4.79E+02	4.77E+02	C23H44N07P	[M+H]+	LysoPE 18:2(2n isomer)	Lipids	LPE	-	A	1.18E+04	4.06E+04	1.05E+05	2.17E+04	1.89E+04	2.09E+04	5.13E+04	8.88E+04	5.64E+04	4.82E+04	5.43E+04	5.27E+04	--	--
Hmjp003123	4.79E+02	4.78E+02	C21H18013	[M+H]+	Quercetin-O-glucuronate	Flavonoids	Flavonols	-	B	3.08E+07	1.19E+07	1.08E+07	8.62E+06	2.01E+07	9.68E+06	1.09E+07	1.56E+07	1.33E+07	2.03E+07	2.13E+07	1.53E+07	--	--
pmm0374	4.77E+02	4.78E+02	C22H22012	[M-H]-	2,6-Dimethyl-7-octene-2,3,6-triol	Flavonoids	Flavonoid	5041-82-7	A	9.00E+05	6.70E+05	1.86E+06	2.70E+05	1.29E+06	4.11E+05	3.36E+05	2.07E+05	3.97E+05	5.74E+05	1.36E+06	8.40E+05	--	--
Hmpp003242	4.79E+02	4.78E+02	C22H22012	[M+H]+	Isorhamnetin-3-O-β-D-glucoside	Flavonoids	Flavonols	-	A	5.05E+06	3.41E+06	8.21E+06	2.03E+06	4.60E+06	1.69E+06	1.56E+06	1.77E+06	2.75E+06	4.40E+06	4.04E+06	3.64E+06	--	--
Hmcp002207	4.79E+02	4.78E+02	C22H22012	[M+H]+	O-β-D-glucopyranoside	Flavonoids	Flavonols	-	A	5.53E+06	3.59E+06	6.92E+06	2.19E+06	4.76E+06	2.14E+06	1.68E+06	1.72E+06	2.18E+06	4.27E+06	3.52E+06	4.10E+06	--	--
pmb0856	4.80E+02	4.79E+02	C23H46N07P	[M+H]+	LysoPE 18:1(2n isomer)	Lipids	LPE	-	B	2.70E+04	1.51E+05	2.87E+05	1.35E+05	8.09E+04	8.97E+04	2.09E+05	3.33E+05	2.13E+05	1.79E+05	1.82E+05	1.76E+05	--	--
mws0289	4.78E+02	4.79E+02	C23H46N07P	[M-H]-	LysoPE 18:1	Lipids	LPE	89576-29-4	A	1.58E+04	7.67E+04	1.56E+05	3.93E+04	2.49E+04	3.62E+04	7.12E+04	1.40E+05	6.35E+04	7.58E+04	7.04E+04	7.16E+04	--	--
Lmmp001947	4.81E+02	4.80E+02	C21H20013	[M+H]+	Gossypetin 3-glucoside	Flavonoids	Flavonols	-	B	1.68E+05	1.01E+05	2.42E+05	4.98E+04	1.60E+05	7.66E+04	4.07E+04	5.21E+04	5.99E+04	1.22E+05	1.10E+05	1.13E+05	--	--
Hmln001933	4.79E+02	4.80E+02	C21H20013	[M-H]-	Myricetin 3-O-galactoside	Flavonoids	Flavonoid	-	B	4.25E+05	1.62E+05	2.28E+05	1.10E+05	2.15E+05	1.33E+05	6.57E+04	1.23E+05	7.14E+04	1.39E+05	1.63E+05	1.54E+05	--	--

Lmln001856	4.79E+02	4.80E+02	C21H20O13	[M-H]-	5,7-Dihydroxy-4-oxo-2-(3,4,5-trihydroxyphenyl)-4H-chromen-3-yl-β-D-	allopyranoside	Others	Others	-	B	3.46E+05	3.63E+05	2.35E+05	1.33E+05	1.84E+05	1.28E+05	7.38E+04	1.26E+05	1.10E+05	2.26E+05	2.20E+05	1.50E+05	--	--
pmb2319	4.82E+02	4.81E+02	C23H48N07P	[M+H]+	LysoPC 15:0	Lipids	LPC	-	B	1.51E+04	1.92E+04	3.86E+04	2.71E+04	1.91E+04	2.36E+04	4.38E+04	5.71E+04	4.98E+04	3.43E+04	3.33E+04	3.29E+04	--	--	
Li512114	4.85E+02	4.86E+02	C31H50O4	[M-H]-	Ursolic acid-OCH3	Terpenoids	Triterpene	-	A	8.05E+04	4.54E+04	3.88E+04	4.05E+04	5.66E+04	3.02E+04	4.22E+04	3.21E+04	3.94E+04	4.75E+04	5.58E+04	5.64E+04	--	--	
pmb0736	4.93E+02	4.92E+02	C23H24O12	[M+H]+	Tricin 7-O-hexoside	Flavonoids	Flavonoid	-	B	2.21E+04	2.68E+04	2.54E+04	2.96E+04	3.55E+04	1.94E+04	2.01E+04	4.15E+04	1.96E+04	3.66E+04	3.53E+04	2.52E+04	--	--	
Hmcp002268	4.93E+02	4.92E+02	C23H24O12	[M+H]+	Limocitrin 3-rhamnoside	Flavonoids	Flavonoid	-	B	1.76E+04	1.62E+04	2.47E+04	3.27E+04	2.44E+04	1.77E+04	2.86E+04	3.28E+04	1.76E+04	4.22E+04	2.73E+04	3.10E+04	--	--	
pme0444	4.93E+02	4.93E+02	C23H25O12+	[M]+	Malvidin 3-O-glucoside (Oenin)	Flavonoids	Anthocyanins	18470-06-9	A	2.68E+06	9.90E+05	7.25E+06	5.66E+05	2.48E+06	2.13E+06	5.48E+05	1.46E+06	1.77E+06	2.17E+06	2.51E+06	2.17E+06	C12140	ko00942	
pme0443	4.93E+02	4.93E+02	C23H25O12+	[M]+	Malvidin 3-O-galactoside (Primulin)	Flavonoids	Anthocyanins	30113-37-2	A	3.45E+06	1.26E+06	8.68E+06	7.44E+05	3.87E+06	3.00E+06	6.34E+05	1.76E+06	2.21E+06	3.02E+06	3.15E+06	2.90E+06	--	--	
pmp001270	4.94E+02	4.93E+02	C24H48N07P	[M+H]+	LysoPC(16:1)	Lipids	LPC	-	B	1.74E+04	3.20E+04	4.53E+04	4.22E+04	4.00E+04	4.06E+04	9.71E+04	9.86E+04	6.77E+04	5.60E+04	4.63E+04	5.31E+04	--	--	
Hmlp002821	4.95E+02	4.94E+02	C21H8O14	[M+H]+	Myricetin-O-glucuronate	Flavonoids	Flavonols	-	A	3.80E+05	9.39E+04	7.53E+04	6.74E+04	1.09E+05	4.70E+04	3.73E+04	9.16E+04	7.85E+04	1.56E+05	1.32E+05	1.34E+05	--	--	
pmd0132	4.96E+02	4.95E+02	C24H50N07P	[M+H]+	LysoPC 16:0(2n isomer)	Lipids	LPC	-	A	1.52E+06	2.68E+06	5.30E+06	2.62E+06	1.93E+06	2.53E+06	4.61E+06	5.28E+06	4.32E+06	3.54E+06	3.49E+06	3.43E+06	--	--	
pmb0855	4.96E+02	4.95E+02	C24H50N07P	[M+H]+	LysoPC 16:0	Lipids	LPC	17364-16-8	A	1.44E+06	2.46E+06	5.08E+06	2.41E+06	1.82E+06	2.30E+06	4.55E+06	4.89E+06	4.26E+06	3.23E+06	3.46E+06	3.36E+06	--	--	
mws1589	5.03E+02	5.04E+02	C18H32O16	[M-H]-	Panose	Others	Saccharides and Alcohols	33401-87-5	B	4.85E+04	4.08E+04	3.20E+04	4.11E+04	4.66E+04	4.27E+04	3.81E+04	4.86E+04	3.99E+04	3.87E+04	4.06E+04	4.25E+04	C00713	--	
pme0500	5.03E+02	5.04E+02	C18H32O16	[M-H]-	Melezitose	Others	Saccharides and Alcohols	597-12-6	B	1.36E+04	1.33E+04	1.46E+04	1.05E+04	2.03E+04	1.62E+04	1.49E+04	1.45E+04	8.49E+03	9.53E+03	1.37E+04	1.26E+04	--	--	
Hmcp002187	5.09E+02	5.08E+02	C23H24O13	[M+H]+	Limocitrin 3-galactoside	Flavonoids	Flavonoid	-	B	8.59E+04	2.47E+04	1.06E+05	3.44E+04	5.95E+04	3.38E+04	2.36E+04	3.14E+04	4.04E+04	4.45E+04	5.28E+04	5.13E+04	--	--	
pmb2406	5.10E+02	5.09E+02	C25H52N07P	[M+H]+	LysoPC 17:0	Lipids	LPC	-	B	8.04E+03	1.30E+04	2.49E+04	1.44E+04	1.26E+04	1.25E+04	2.51E+04	3.18E+04	2.62E+04	1.91E+04	1.97E+04	1.99E+04	--	--	
pmb0854	5.18E+02	5.17E+02	C26H48N07P	[M+H]+	LysoPC 18:3	Lipids	LPC	-	B	1.13E+05	2.16E+05	4.48E+05	1.10E+05	9.24E+04	1.18E+05	2.42E+05	3.18E+05	2.91E+05	2.14E+05	2.49E+05	2.49E+05	--	--	
pmb0865	5.18E+02	5.17E+02	C26H48N07P	[M+H]+	LysoPC 18:3(2n isomer)	Lipids	LPC	-	A	3.32E+05	8.96E+05	1.53E+06	5.65E+05	3.24E+05	5.02E+05	8.86E+05	1.25E+06	9.86E+05	8.34E+05	8.01E+05	8.13E+05	--	--	
pmp001273	5.20E+02	5.19E+02	C26H50N07P	[M+H]+	LysoPC(18:2)	Lipids	LPC	-	A	3.65E+05	6.68E+05	1.67E+06	4.74E+05	4.98E+05	5.40E+05	1.34E+06	1.70E+06	1.29E+06	8.68E+05	9.69E+05	9.75E+05	--	--	
pmp000682	5.38E+02	5.20E+02	C26H32O11	[M+NH4]+	Matairesinoideside	Lignans and Coumarins	Lignans	23202-85-9	B	8.19E+05	5.70E+05	7.76E+05	5.42E+05	8.07E+05	5.15E+05	8.88E+05	5.78E+05	7.12E+05	7.35E+05	8.03E+05	6.62E+05	--	--	
Rfmb25703	5.19E+02	5.20E+02	C26H32O11	[M-H]-	Pinoresinol-Hexose	Lignans and Coumarins	Lignans	-	B	9.00E+00	3.07E+05	2.63E+05	2.25E+05	5.77E+05	3.00E+05	8.09E+05	8.03E+05	9.00E+00	4.73E+05	3.97E+05	5.56E+05	--	--	
pmp001251	5.20E+02	5.20E+02	C26H51N07P+	[M]+	PC(18:2)isomer	Lipids	PC	-	A	9.34E+05	2.45E+06	4.68E+06	2.10E+06	1.43E+06	1.78E+06	4.21E+06	5.46E+06	3.88E+06	3.09E+06	3.10E+06	3.20E+06	--	--	
pmp001250	5.20E+02	5.20E+02	C26H51N07P+	[M]+	PC(18:2)	Lipids	PC	-	A	3.93E+05	6.65E+05	1.69E+06	4.93E+05	4.89E+05	5.21E+05	1.31E+06	1.67E+06	1.24E+06	9.23E+05	1.01E+06	9.91E+05	--	--	
pmp001281	5.22E+02	5.21E+02	C26H52N07P	[M+H]+	LysoPC(18:1)	Lipids	LPC	-	A	9.56E+04	2.08E+05	3.59E+05	1.48E+05	1.46E+05	1.75E+05	2.96E+05	5.30E+05	3.07E+05	2.50E+05	2.68E+05	2.69E+05	--	--	
pmp001286	5.24E+02	5.23E+02	C26H54N07P	[M+H]+	LysoPC(18:0)	Lipids	LPC	-	B	1.14E+05	2.24E+05	3.26E+05	1.87E+05	1.49E+05	2.03E+05	3.42E+05	3.59E+05	3.44E+05	2.31E+05	2.51E+05	2.56E+05	--	--	
pmd0136	5.24E+02	5.23E+02	C26H54N07P	[M+H]+	LysoPC 18:0	Lipids	LPC	-	B	1.34E+05	2.30E+05	3.75E+05	1.99E+05	1.56E+05	2.21E+05	3.66E+05	3.91E+05	3.33E+05	2.65E+05	2.57E+05	2.54E+05	--	--	

mws0126	5.24E+02	5.23E+02	C26H54N O7P	[M+H] ⁺	1-Stearoyl-sn-glycero-3-phosphocholine	Lipids	LPC	19420-57-6	B	1.19E+05	2.22E+05	3.51E+05	1.85E+05	1.55E+05	2.15E+05	3.49E+05	3.96E+05	3.44E+05	2.48E+05	2.60E+05	2.58E+05	--	--
pmp001282	5.44E+02	5.43E+02	C28H50N O7P	[M+H] ⁺	Propyl2-(trimethylammonio)ethyl phosphate	Others	Others	-	B	8.65E+03	2.19E+04	3.32E+04	1.25E+04	1.33E+04	1.75E+04	2.64E+04	4.50E+04	2.71E+04	2.19E+04	2.38E+04	2.20E+04	--	--
pmp000589	5.51E+02	5.50E+02	C24H22O 15	[M+H] ⁺	Quercetin-7-O-(6'-O-malonyl)-β-D-glucoside	Flavonoids	Flavonols	-	B	3.42E+04	2.11E+04	1.87E+04	1.57E+04	3.55E+04	1.74E+04	2.14E+04	3.48E+04	2.94E+04	3.11E+04	3.00E+04	3.09E+04	--	--
Hmln002189	5.49E+02	5.50E+02	C24H22O 15	[M-H] ⁻	Quercetin 3-O-(6''-O-malonyl)-galactoside	Flavonoids	Flavonols	-	B	1.42E+04	9.00E+00	7.40E+03	5.68E+03	1.54E+04	2.86E+03	9.00E+00	1.37E+04	8.53E+03	1.25E+04	1.25E+04	1.17E+04	--	--
Zmhn001414	5.51E+02	5.52E+02	C26H32O 13	[M-H] ⁻	Resveratrol-O-diglucoside	Others	Stilbene	-	A	9.00E+00	2.56E+04	3.87E+04	9.95E+03	9.00E+00	8.32E+03	5.33E+03	6.00E+03	2.43E+04	2.19E+04	9.98E+03	1.83E+04	--	--
pmb2922	5.65E+02	5.66E+02	C15H24N 2O17P2	[M-H] ⁻	Uridine 5'-diphospho-D-glucose	Nucleotides and derivatives	Nucleotides and derivatives	133-89-1	B	2.38E+06	1.93E+06	1.90E+06	1.74E+06	2.34E+06	2.13E+06	1.40E+06	1.23E+06	1.46E+06	2.21E+06	2.43E+06	2.09E+06	C00029	ko00053,ko00240,ko00500,ko00520,ko00561,ko00908,ko01100
pme0431	5.77E+02	5.76E+02	C30H24O 12	[M+H] ⁺	Procyanidin A1	Tannins	Proanthocyanidins	103883-03-0	B	6.47E+03	7.79E+03	1.42E+04	1.57E+04	3.51E+04	1.85E+04	3.09E+04	3.92E+04	6.54E+04	3.75E+04	3.06E+04	3.58E+04	--	--
pme0433	5.77E+02	5.76E+02	C30H24O 12	[M+H] ⁺	Procyanidin A2	Tannins	Proanthocyanidins	41743-41-3	B	9.00E+00	1.06E+04	1.00E+04	1.21E+04	2.64E+04	1.88E+04	4.17E+04	4.25E+04	7.87E+04	2.51E+04	2.85E+04	2.96E+04	C10237	--
pmb0837	5.77E+02	5.76E+02	C30H24O 12	[M+H] ⁺	Procyanidin A3	Tannins	Proanthocyanidins	86631-39-2	B	1.57E+05	2.58E+05	1.53E+05	2.61E+05	2.07E+05	2.02E+05	1.94E+05	1.85E+05	2.20E+05	2.60E+05	2.42E+05	2.54E+05	--	--
pme0368	5.79E+02	5.78E+02	C27H30O 14	[M+H] ⁺	Apigenin 7-rutinoside(Isorhoifolin)	Flavonoids	Flavonoid	552-57-8	B	2.38E+05	2.92E+05	3.13E+05	1.62E+05	2.93E+05	1.34E+05	7.50E+04	1.13E+05	1.65E+05	2.13E+05	1.90E+05	2.20E+05	--	--
pnn001667	5.77E+02	5.78E+02	C30H26O 12	[M-H] ⁻	Procyanidin B4	Tannins	Proanthocyanidins	29106-51-2	A	2.61E+04	3.66E+04	1.27E+04	3.60E+04	3.31E+04	2.97E+04	1.01E+04	2.23E+04	2.33E+04	4.97E+04	3.40E+04	3.80E+04	C10238	--
pme0434	5.77E+02	5.78E+02	C30H26O 12	[M-H] ⁻	Procyanidin B2	Tannins	Proanthocyanidins	29106-49-8	A	2.76E+06	4.92E+06	2.32E+06	4.10E+06	2.92E+06	2.58E+06	1.82E+06	2.23E+06	2.91E+06	2.84E+06	3.50E+06	3.79E+06	C17639	--
pme0436	5.77E+02	5.78E+02	C30H26O 12	[M-H] ⁻	Procyanidin B3	Tannins	Proanthocyanidins	23567-23-9	A	2.80E+06	4.76E+06	2.33E+06	3.48E+06	2.48E+06	2.67E+06	2.04E+06	1.98E+06	2.35E+06	3.60E+06	3.38E+06	3.57E+06	--	--
mws0836	5.77E+02	5.78E+02	C30H26O 12	[M-H] ⁻	Procyanidin B1	Tannins	Proanthocyanidins	20315-25-7	A	1.91E+06	3.39E+06	1.78E+06	2.67E+06	2.10E+06	2.05E+06	1.54E+06	1.59E+06	2.71E+06	2.25E+06	2.50E+06	2.11E+06	--	--
Hmmp001656	5.79E+02	5.78E+02	C27H31O 14	[M+H] ⁺	Pelargonin-O-rutinoside	Flavonoids	Anthocyanins	-	B	7.45E+03	2.28E+04	1.38E+04	1.56E+04	1.69E+04	1.05E+04	1.29E+04	1.25E+04	1.57E+04	1.72E+04	1.40E+04	1.64E+04	--	--
Hmcp002029	5.81E+02	5.80E+02	C26H28O 15	[M+H] ⁺	Kaempferol-O-pentoside	Flavonoids	Flavonols	-	A	1.31E+05	9.00E+00	9.00E+00	9.00E+00	1.91E+04	9.00E+00	9.00E+00	1.60E+04	9.65E+03	2.25E+04	2.41E+04	2.24E+04	--	--
mws1290	5.93E+02	5.94E+02	C30H26O 13	[M-H] ⁻	Tiliroside	Flavonoids	Flavonols	20316-62-5	B	3.96E+03	9.51E+03	6.63E+03	8.57E+03	1.23E+04	7.44E+03	2.85E+03	3.08E+03	4.53E+03	1.00E+04	1.10E+04	1.17E+04	C17140	--
GQ512005	5.95E+02	5.94E+02	C27H30O 15	[M+H] ⁺	Kaempferol-3-O-glucoside-7-O-rhamnoside	Flavonoids	Flavonols	-	B	1.71E+05	9.00E+00	9.00E+00	9.00E+00	2.57E+04	8.72E+03	6.97E+03	1.57E+04	8.31E+03	3.62E+04	2.98E+04	2.61E+04	--	--
pme1605	5.93E+02	5.94E+02	C27H30O 15	[M-H] ⁻	Kaempferol 3-O-robinobioside(Biorobin)	Flavonoids	Flavonols	17297-56-2	A	3.87E+05	6.91E+05	3.11E+05	3.53E+05	5.29E+05	3.86E+05	1.47E+05	2.40E+05	2.28E+05	4.38E+05	3.80E+05	3.78E+05	--	--
pmp000593	5.95E+02	5.94E+02	C27H30O 15	[M+H] ⁺	Luteolin-7-O-rutinoside	Flavonoids	Flavonoid	3563-98-2	B	2.11E+06	1.30E+05	6.96E+04	5.79E+04	2.96E+05	8.58E+04	6.36E+04	1.57E+05	9.48E+04	3.96E+05	3.59E+05	3.61E+05	--	--
pme0369	5.93E+02	5.94E+02	C27H30O 15	[M-H] ⁻	Kaempferol 3-O-rutinoside(Nicotiflorin)	Flavonoids	Flavonols	17650-84-9	A	3.53E+05	3.73E+05	2.20E+05	3.96E+05	7.11E+05	2.66E+05	1.18E+05	2.16E+05	1.79E+05	3.83E+05	3.08E+05	3.50E+05	C21833	ko00944,ko01110

Lnrp002296	5.95E+02	5.94E+02	C27H30O15	[M+H] ⁺	Kaempferol glc-rha	Flavonoids	Flavonols	-	A	2.80E+07	2.97E+07	2.47E+07	3.03E+07	4.61E+07	2.26E+07	1.25E+07	2.00E+07	1.39E+07	2.89E+07	2.61E+07	3.00E+07	--	--
Lmbp003230	5.95E+02	5.94E+02	C27H30O15	[M+H] ⁺	neohesperidosid e	Flavonoids	Flavonols	32602-81-6	A	3.25E+07	3.10E+07	2.28E+07	3.02E+07	4.72E+07	2.20E+07	1.03E+07	1.81E+07	1.50E+07	3.32E+07	2.62E+07	2.79E+07	--	--
pme1773	5.95E+02	5.95E+02	C27H31O15+	[M] ⁺	Cyanidin 3-O- rutinoside (Keracyanin)	Flavonoids	Anthocyanins	28338-59-2	B	1.41E+05	1.63E+05	7.98E+04	2.01E+05	8.44E+04	1.27E+05	9.01E+04	7.89E+04	2.66E+04	1.47E+05	1.16E+05	1.20E+05	C08620	ko00942
pme1793	5.95E+02	5.95E+02	C27H31O15+	[M] ⁺	Pelargonidin 3,5-diglucoside	Flavonoids	Anthocyanins	17334-58-6	B	8.41E+04	7.37E+04	5.55E+04	6.84E+04	5.31E+04	5.06E+04	3.77E+04	6.17E+04	3.99E+04	6.72E+04	5.75E+04	4.30E+04	C08725	ko00942
Hmcp001447	5.97E+02	5.96E+02	C26H28O16	[M+H] ⁺	Quercetin-O- Hexoside-O- Pentoside	Flavonoids	Flavonols	-	A	3.09E+04	2.49E+04	1.46E+04	1.48E+04	1.72E+04	9.37E+03	1.13E+04	9.02E+03	7.09E+03	2.09E+04	2.28E+04	1.81E+04	--	--
pmb3002	6.07E+02	6.08E+02	C28H32O15	[M-H] ⁻	Chrysoeriol 7- O-rutinoside	Flavonoids	Flavonoid	-	A	1.11E+06	2.38E+06	3.21E+06	1.76E+06	2.82E+06	1.17E+06	6.85E+05	1.45E+06	2.93E+06	1.74E+06	2.10E+06	1.82E+06	--	--
mws1661	6.09E+02	6.08E+02	C28H32O15	[M+H] ⁺	Diosmin	Flavonoids	Flavonoid	520-27-4	B	4.20E+06	6.60E+06	7.32E+06	5.75E+06	7.25E+06	4.02E+06	2.44E+06	4.98E+06	5.40E+06	6.82E+06	6.47E+06	6.84E+06	C10039	--
pmb0665	6.11E+02	6.10E+02	C27H30O16	[M+H] ⁺	Luteolin 8-C- hexosyl-O- hexoside	Flavonoids	Flavonoid	-	B	6.18E+05	1.44E+05	8.47E+04	7.81E+04	2.56E+05	7.67E+04	9.71E+04	1.19E+05	1.26E+05	2.14E+05	1.94E+05	1.84E+05	--	--
Li512117	6.11E+02	6.10E+02	C27H30O16	[M+H] ⁺	Quercetin 3-O- rhanosylgalacto side	Flavonoids	Flavonols	-	B	5.16E+05	1.81E+05	8.10E+04	8.77E+04	2.74E+05	1.01E+05	1.06E+05	1.51E+05	8.88E+04	2.16E+05	1.86E+05	2.06E+05	--	--
pmm001583	6.09E+02	6.10E+02	C27H30O16	[M-H] ⁻	Bioquercetin	Flavonoids	Flavonols	52525-35-6	A	6.82E+06	1.24E+06	8.08E+05	7.44E+05	2.66E+06	1.06E+06	8.46E+05	1.65E+06	1.28E+06	3.25E+06	2.25E+06	1.99E+06	--	--
mws0059	6.09E+02	6.10E+02	C27H30O16	[M-H] ⁻	Rutin	Flavonoids	Flavonols	153-18-4	A	4.51E+06	1.14E+06	5.90E+05	7.04E+05	1.95E+06	5.85E+05	7.93E+05	1.33E+06	1.09E+06	1.78E+06	1.16E+06	1.29E+06	--	--
Lmyp004516	6.11E+02	6.10E+02	C30H26O14	[M+H] ⁺	(6"-trans-p- Coumaroyl)-β- D- glucopyranosid e	Flavonoids	Flavonols	-	A	9.71E+03	1.89E+04	2.47E+04	1.32E+04	2.48E+04	1.22E+04	6.13E+03	1.69E+04	1.89E+04	1.95E+04	1.92E+04	2.13E+04	--	--
Lmyp004052	6.11E+02	6.10E+02	C30H26O14	[M+H] ⁺	Quercetin 3-O- (6"-trans-p- Coumaroyl)-β- D- galactopyranosi de	Flavonoids	Flavonols	-	A	6.56E+04	1.76E+05	1.79E+05	7.70E+04	7.97E+04	4.88E+04	2.20E+04	7.47E+04	8.16E+04	1.10E+05	1.12E+05	8.96E+04	--	--
Hmmp002336	6.11E+02	6.10E+02	C30H26O14	[M+H] ⁺	Quercetin-O- feruloyl- Pentoside	Flavonoids	Flavonols	-	A	1.51E+07	4.97E+06	2.08E+06	2.93E+06	7.73E+06	3.36E+06	2.87E+06	4.59E+06	3.73E+06	6.83E+06	6.14E+06	7.12E+06	--	--
Lnrp002462	6.11E+02	6.10E+02	C27H30O16	[M+H] ⁺	quercetin galactoside- rhamnoside	Flavonoids	Flavonols	-	A	8.80E+05	1.50E+06	1.84E+06	1.14E+06	1.69E+06	7.52E+05	6.17E+05	1.10E+06	1.23E+06	1.48E+06	1.43E+06	1.44E+06	--	--
pme0001	6.09E+02	6.10E+02	C28H34O15	[M-H] ⁻	O- neohesperidosid e(Neohesperidi n)	Flavonoids	Dihydroflavone	13241-33-3	A	2.03E+04	4.14E+04	6.11E+04	4.09E+04	2.15E+04	2.40E+04	1.83E+04	3.32E+04	1.30E+04	4.59E+04	3.63E+04	3.76E+04	C09806	ko00941
mws0036	6.09E+02	6.10E+02	C28H34O15	[M-H] ⁻	Hesperidin	Flavonoids	Dihydroflavone	520-26-3	A	1.49E+06	2.83E+05	1.69E+05	1.63E+05	6.69E+05	1.98E+05	2.69E+05	3.11E+05	2.84E+05	6.64E+05	3.33E+05	3.40E+05	C09755	--
Lmbp003805	6.11E+02	6.11E+02	C27H31O16+	[M] ⁺	Delphinidin-3- rutinoside	Flavonoids	Flavonoid	15674-58-5	A	5.84E+04	1.52E+05	1.56E+05	6.99E+04	8.66E+04	5.40E+04	2.52E+04	5.40E+04	6.82E+04	9.99E+04	8.60E+04	8.75E+04	C16315	ko00942
mws4134	6.11E+02	6.12E+02	C20H32N6O12S2	[M-H] ⁻	Oxidized Glutathione	Amino acids and derivatives	Amino acids and derivatives	121-24-4	B	1.35E+05	9.29E+04	9.02E+04	2.22E+04	1.89E+04	1.98E+04	2.99E+04	1.88E+04	1.95E+04	6.97E+04	6.66E+04	5.27E+04	--	--
pmb0628	6.13E+02	6.12E+02	C27H32O16	[M+H] ⁺	Eriodictiol C- hexosyl-O- hexoside	Flavonoids	Dihydroflavone	-	B	6.06E+04	8.55E+04	3.77E+04	6.54E+04	1.16E+05	5.45E+04	4.81E+04	4.53E+04	4.98E+04	7.01E+04	6.60E+04	6.30E+04	--	--

Zmxp002867	6.25E+02	6.24E+02	C28H32O16	[M+H] ⁺	Chrysoeriol-di-O-glucoside	Flavonoids	Flavonoid	-	B	8.25E+05	2.11E+06	1.41E+06	1.68E+06	1.99E+06	9.73E+05	1.32E+06	2.66E+06	1.84E+06	1.51E+06	1.93E+06	3.13E+06	--	--
Lmmp002963	6.25E+02	6.24E+02	C28H32O16	[M+H] ⁺	Methylquercetin glu-rhamnoside	Flavonoids	Flavonols	-	B	3.60E+05	1.51E+05	3.85E+05	1.08E+05	6.52E+05	1.66E+05	6.43E+04	1.47E+05	1.42E+05	2.40E+05	2.80E+05	2.90E+05	--	--
pmb0614	6.25E+02	6.25E+02	C28H33O16 ⁺	[M] ⁺	Peonidin 3,5-O-digluconide chloride	Flavonoids	Anthocyanins	47851-83-2	B	1.22E+05	2.32E+05	9.32E+05	6.24E+04	8.13E+04	6.42E+04	4.78E+04	5.48E+04	1.97E+05	1.91E+05	1.81E+05	2.05E+05	--	--
pmp000596	6.27E+02	6.26E+02	C27H30O17	[M+H] ⁺	Quercetin 3,7-bis-O-β-D-glucoside-6-	Flavonoids	Flavonols	-	B	6.02E+05	4.00E+05	4.38E+05	4.03E+05	4.91E+05	3.89E+05	2.30E+05	2.23E+05	1.88E+05	4.26E+05	3.55E+05	2.91E+05	--	--
pmp001311	6.27E+02	6.26E+02	C27H30O17	[M+H] ⁺	Hydroxykaempferol-7,6-O-Digluconide	Flavonoids	Flavonols	-	B	6.92E+05	4.41E+05	5.07E+05	4.35E+05	5.61E+05	5.68E+05	2.97E+05	4.60E+05	3.20E+05	5.76E+05	5.98E+05	4.85E+05	--	--
Lmhp002613	6.27E+02	6.26E+02	C27H30O17	[M+H] ⁺	Myricetin-O-glucoside-rhamnoside	Flavonoids	Flavonols	-	B	4.79E+04	1.44E+04	1.01E+04	5.73E+03	7.18E+03	9.09E+03	1.10E+04	6.78E+03	6.87E+03	1.81E+04	1.92E+04	1.55E+04	--	--
pmb0645	6.27E+02	6.26E+02	C28H34O16	[M+H] ⁺	6-C-Hexosyl-hesperetin O-hexoside	Flavonoids	Flavonoid carbonoside	-	B	2.16E+05	2.29E+05	2.81E+05	2.56E+05	2.79E+05	2.70E+05	1.39E+05	2.26E+05	1.66E+05	2.50E+05	2.29E+05	2.21E+05	--	--
pmb0618	6.27E+02	6.26E+02	C28H34O16	[M+H] ⁺	8-C-Hexosyl-hesperetin O-hexoside	Flavonoids	Flavonoid carbonoside	-	B	2.19E+05	1.20E+05	1.93E+05	1.67E+05	2.01E+05	1.50E+05	1.13E+05	9.40E+04	1.07E+05	1.77E+05	1.67E+05	1.69E+05	--	--
Hmyp007792	6.36E+02	6.35E+02	C32H62N9O9P	[M+H] ⁺	PE(oxo-11:0/16:0)	Lipids	Glycerol ester	-	B	4.64E+04	2.99E+05	3.31E+05	1.51E+05	3.87E+04	7.23E+04	9.82E+04	2.01E+05	8.09E+04	1.52E+05	1.53E+05	1.52E+05	--	--
pmb3043	6.37E+02	6.38E+02	C29H34O16	[M-H] ⁻	Tricin 5-O-rutinoside	Flavonoids	Flavonoid	-	B	1.92E+04	1.89E+04	5.21E+04	1.09E+04	1.62E+04	2.92E+04	6.33E+03	2.58E+04	3.03E+04	3.96E+04	3.55E+04	3.23E+04	--	--
Hmcp003086	6.39E+02	6.38E+02	C29H34O16	[M+H] ⁺	Tricin-O-Hexoside-O-rhamnoside	Flavonoids	Flavonoid	-	B	1.20E+06	6.04E+05	1.89E+06	3.56E+05	1.63E+06	7.43E+05	3.24E+05	1.03E+06	1.15E+06	1.16E+06	1.23E+06	1.23E+06	--	--
Hmcp002249	6.39E+02	6.38E+02	C29H34O16	[M+H] ⁺	Limocitrin-O-rhamnoside-O-rhamnoside	Flavonoids	Flavonoid	-	A	1.07E+06	5.58E+05	2.38E+06	3.70E+05	1.67E+06	8.71E+05	3.41E+05	9.90E+05	1.15E+06	1.20E+06	1.16E+06	1.19E+06	--	--
pmb0530	6.64E+02	6.63E+02	C21H27N7O14P2	[M+H] ⁺	Nicotinic acid adenine dinucleotide	Nucleotides and derivatives	Nucleotides and derivatives	53-84-9	B	1.02E+05	1.46E+05	1.21E+05	2.39E+05	2.05E+05	2.39E+05	1.55E+05	1.96E+05	1.61E+05	1.94E+05	1.47E+05	1.83E+05	C00003	ko00190,ko00730,ko00760,ko01100
pmm001588	6.65E+02	6.66E+02	C24H42O21	[M-H] ⁻	Nystose	Others	Saccharides and Alcohols	13133-07-8	B	6.28E+04	1.37E+05	1.82E+05	3.78E+04	1.56E+05	4.12E+04	1.60E+05	9.30E+04	1.20E+05	1.30E+05	1.22E+05	6.99E+04	--	--
pme2746	7.84E+02	7.85E+02	C27H33N9O15P2	[M-H] ⁻	Flavin adenine dinucleotide(FAD)	Nucleotides and derivatives	Nucleotides and derivatives	146-14-5	B	3.78E+04	5.22E+04	4.51E+04	2.45E+04	3.06E+04	3.40E+04	2.54E+04	2.79E+04	2.76E+04	3.57E+04	3.73E+04	5.19E+04	C00016	ko00740,ko01100,ko01110
pmp001312	7.89E+02	7.88E+02	C33H40O22	[M+H] ⁺	Hydroxykaempferol-3,7,6-O-triglycoside	Flavonoids	Flavonols	-	B	2.74E+04	6.47E+04	1.16E+05	3.17E+04	1.88E+04	2.05E+04	9.11E+03	1.78E+04	2.77E+04	5.28E+04	3.05E+04	4.11E+04	--	--
pmb0615	7.89E+02	7.88E+02	C34H44O21	[M+H] ⁺	Hesperetin C-hexosyl-O-hexosyl-O-hexoside-6-	Flavonoids	Dihydroflavonol	-	B	2.00E+04	4.51E+04	7.64E+04	1.22E+04	1.52E+04	1.78E+04	6.35E+03	1.02E+04	2.70E+04	2.79E+04	2.73E+04	2.95E+04	--	--
pmp001313	8.03E+02	8.02E+02	C33H38O23	[M+H] ⁺	Hydroxykaempferol-3,6-O-Digluconide-7-O-Glucuronic Acid	Flavonoids	Flavonols	-	B	5.75E+03	1.88E+04	3.32E+04	1.41E+04	4.87E+03	1.16E+04	1.33E+04	9.57E+03	4.64E+04	1.71E+04	1.61E+04	2.07E+04	--	--
pmb2947	8.65E+02	8.66E+02	C45H38O18	[M-H] ⁻	Catechin-catechin-catechin	Tannins	Proanthocyanidins	-	A	1.88E+04	4.19E+04	2.45E+04	3.52E+04	2.44E+04	3.74E+04	1.49E+04	2.37E+04	1.77E+04	4.27E+04	4.57E+04	4.47E+04	--	--

pmp000280	8.67E+02	8.66E+02	C45H38O 18	[M+H] ⁺	Procyanidin C2	Tannins	Proanthocyanid 37064-31- ins	6	A	1.35E+05	1.56E+05	1.70E+05	1.63E+05	1.86E+05	1.26E+05	1.39E+05	1.13E+05	1.94E+05	2.71E+05	2.12E+05	2.46E+05	--	--
pmm001646	8.65E+02	8.66E+02	C45H38O 18	[M-H] ⁻	Procyanidin C1	Tannins	Proanthocyanid 37064-30- ins	5	A	1.88E+04	3.11E+04	1.54E+04	1.25E+04	1.84E+04	2.40E+04	2.32E+04	3.82E+04	2.56E+04	6.32E+04	5.65E+04	4.10E+04	C17624	--