

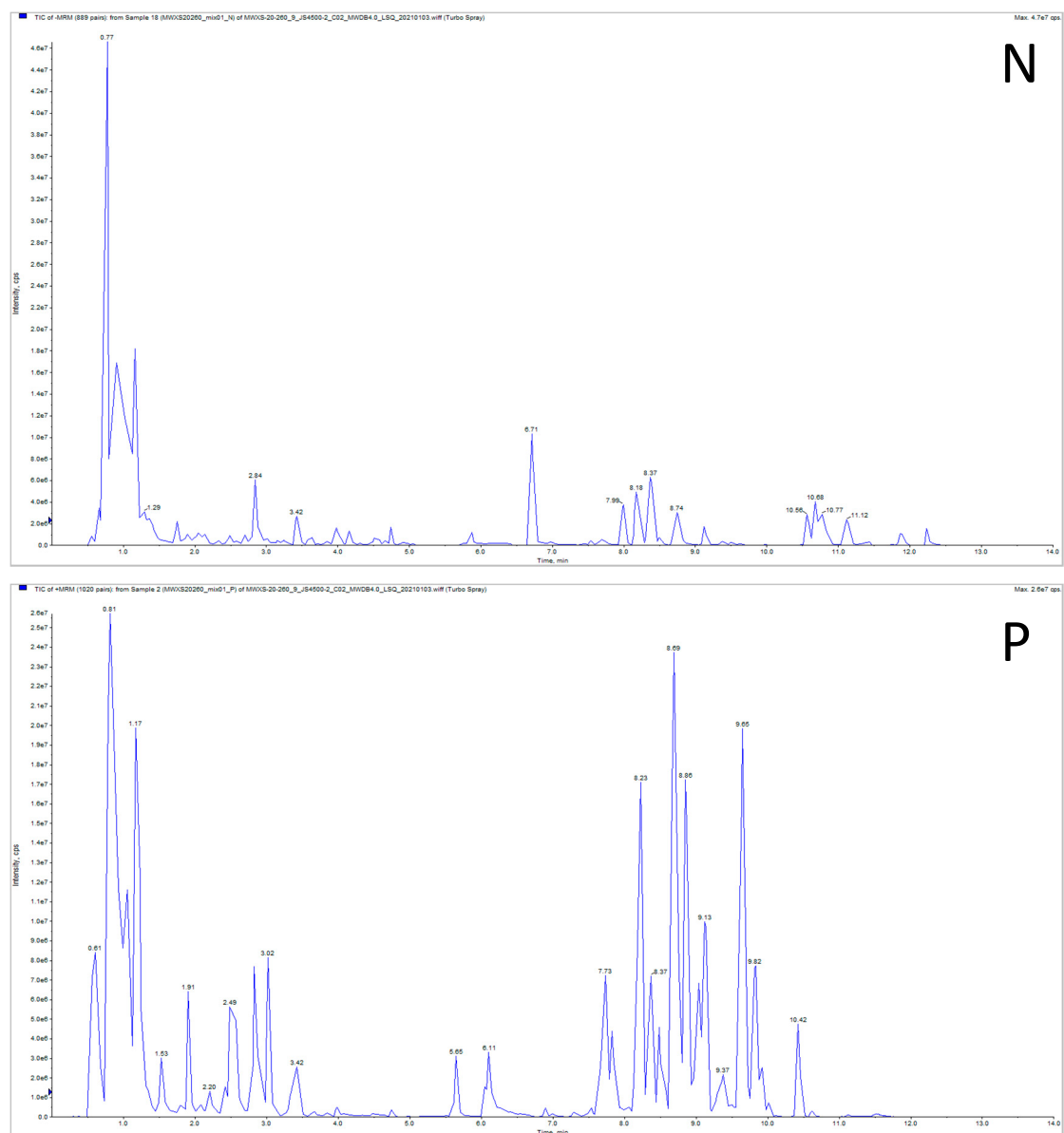


Figure S1 Total ion chromatogram (TIC) of mass spectrometry analysis for pooled samples.

Note: N stands for negative ion mode, P stands for positive ion mode

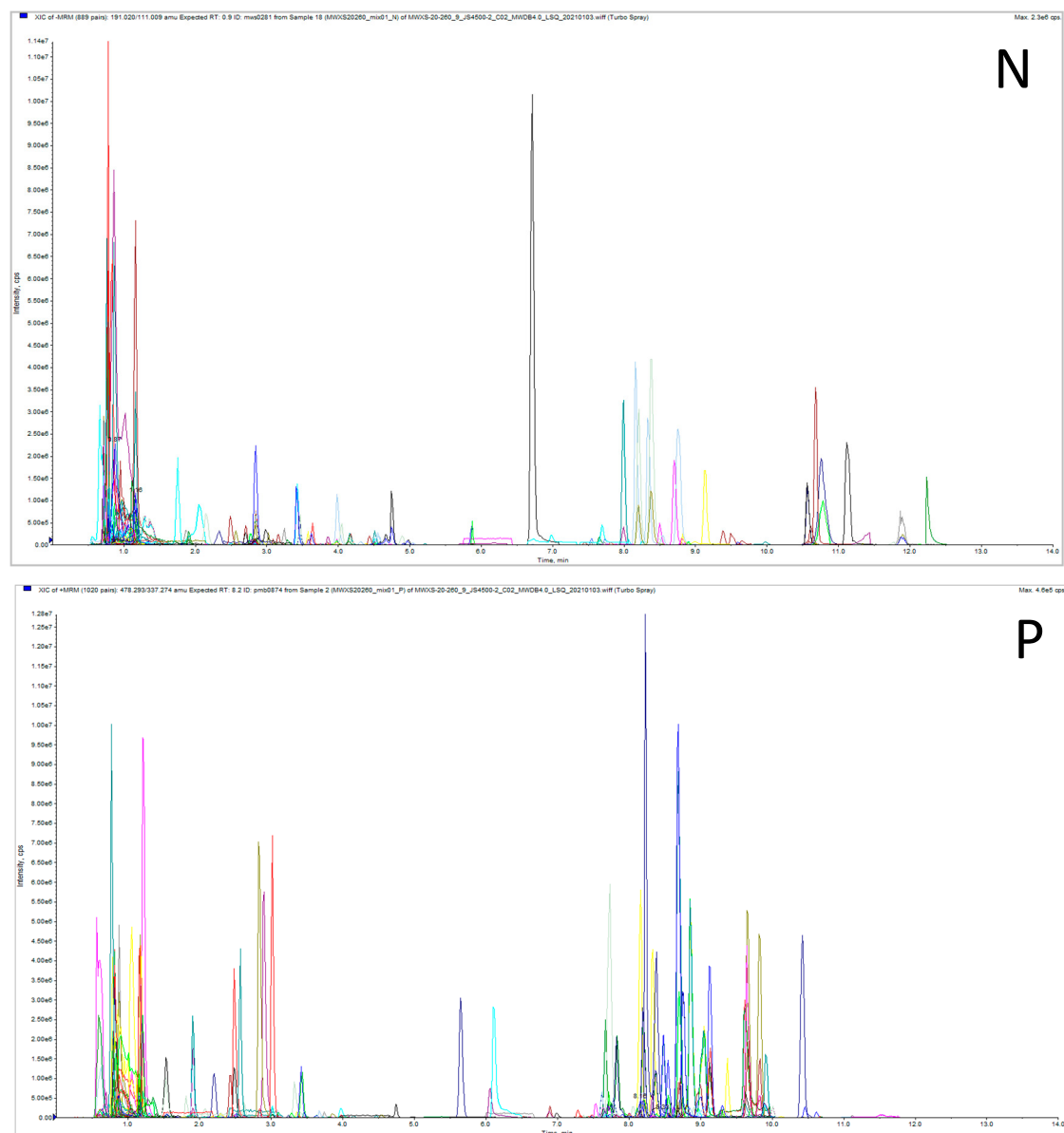


Figure S2 Multiple reaction monitoring (MRM) chromatograms of detected metabolites. Figure

Table S1 Detailed information of 127 representative metabolites used for correlation analysis.

	Index	Q1 (Da)	Q3 (Da)	Molecular Weight (Da)	Ionization model	Compounds	Class I	Class II	CAS	Level	S	L	H
Sugars and sugar alcohols	mws4170	179.0 6	59.01	180.063	[M-H]-	D-Glucose*	Others	Saccharides and Alcohols	14431-43- 7	A	2.20E+ 06	1.28E+ 07	1.20E+ 07
	mws1164	179.0 6	59.01	180.063	[M-H]-	D-Fructose*	Others	Saccharides and Alcohols	7660-25-5	A	2.06E+ 06	1.32E+ 07	1.12E+ 07
	pmf0138	179.0 6	59	180.063	[M-H]-	D-Mannose*	Others	Saccharides and Alcohols	3458-28-4	B	2.19E+ 06	1.33E+ 07	1.08E+ 07
	pmf0139	179.0 6	59	180.063	[M-H]-	D-Galactose*	Others	Saccharides and Alcohols	59-23-4	A	2.25E+ 06	1.33E+ 07	1.12E+ 07
	mws1499	149.0 5	59.01	150.053	[M-H]-	D-Arabinose	Others	Saccharides and Alcohols	10323-20- 3	B	3.87E+ 04	1.79E+ 05	1.47E+ 05
	mws1155	181.0 7	101.0 2	182.079	[M-H]-	D-Mannitol	Others	Saccharides and Alcohols	69-65-8	B	8.63E+ 03	8.07E+ 03	3.23E+ 04
	mws0214	181.0 7	71	182.079	[M-H]-	D-Sorbitol	Others	Saccharides and Alcohols	50-70-4	B	3.27E+ 04	7.00E+ 04	1.79E+ 05
	mws1090	259.0 2	97	260.03	[M-H]-	Glucose-1-phosphate*	Others	Saccharides and Alcohols	59-56-3	A	3.23E+ 06	5.03E+ 06	4.66E+ 06
Organic acids	pme3313	259	97	260.03	[M-H]-	D-Fructose 6-phosphate*	Others	Saccharides and Alcohols	643-13-0	A	3.18E+ 06	5.14E+ 06	4.55E+ 06
	mws0192	117.0 2	73	118.027	[M-H]-	Succinic acid*	Organic acids	Organic acids	110-15-6	A	5.95E+ 06	5.25E+ 06	6.57E+ 06
	mws0376	115	71	116.011	[M-H]-	Fumaric acid	Organic acids	Organic acids	110-17-8	B	8.95E+ 04	1.44E+ 05	1.76E+ 05
	mws0275	133.0 1	71.01	134.022	[M-H]-	L-Malic acid*	Organic acids	Organic acids	97-67-6	A	8.54E+ 05	9.30E+ 05	8.11E+ 05
	mws0281	191.0 2	111.0 1	192.027	[M-H]-	Citric Acid*	Organic acids	Organic acids	77-92-9	A	1.81E+ 07	8.87E+ 06	1.43E+ 07
	pme2380	145.0 1	101	146.022	[M-H]-	α -Ketoglutaric acid	Organic acids	Organic acids	328-50-7	A	6.63E+ 05	4.82E+ 05	1.31E+ 05
	mws0277	191.0 6	85	192.063	[M-H]-	Quinic Acid	Organic acids	Organic acids	77-95-2	A	1.17E+ 07	6.29E+ 06	7.75E+ 06
	Lmgn0001 88	89.02	59.01	90.032	[M-H]-	D-Lactic Acid	Organic acids	Organic acids	10326-41- 7	B	9.00E+ 00	1.69E+ 04	1.17E+ 04
	Zmyn0004 53	191.0 2	111.0 1	192.027	[M-H]-	Isocitric Acid*	Organic acids	Organic acids	320-77-4	A	2.73E+ 07	1.60E+ 07	2.13E+ 07
	pme2589	159.1	87	160.037	[M-H]-	2-Oxoadipic acid	Organic acids	Organic acids	3184-35-8	B	8.04E+ 05	4.53E+ 04	9.00E+ 00
	pme0010	106	60	105.043	[M+H] ⁺	L-Serine	Amino acids and derivatives	Amino acids and derivatives	56-45-1	A	2.77E+ 05	2.19E+ 05	2.90E+ 05
	pme0006	116.0 7	70.1	115.063	[M+H] ⁺	L-Proline	Amino acids and derivatives	Amino acids and derivatives	147-85-3	A	1.25E+ 07	7.43E+ 06	2.07E+ 07
Amino acids	mws0256	118.0 9	72.1	117.079	[M+H] ⁺	L-Valine	Amino acids and derivatives	Amino acids and derivatives	72-18-4	A	8.49E+ 06	1.02E+ 07	3.47E+ 07
	mws0230	120.0 7	74	119.058	[M+H] ⁺	L-Threonine*	Amino acids and derivatives	Amino acids and derivatives	72-19-5	A	1.00E+ 06	8.31E+ 05	2.11E+ 06
	pme0195	120.0 2	62	121.02	[M-H]-	L-Cysteine	Amino acids and derivatives	Amino acids and derivatives	52-90-4	A	4.63E+ 05	4.48E+ 04	1.98E+ 04

Lignans	mws1587	132.1	86	131.095	[M+H] ⁺	L-Norleucine*	Amino acids and derivatives	Amino acids and derivatives	327-57-1	A	2.16E+05	1.20E+05	4.74E+05
	mws0258	132.1	86	131.095	[M+H] ⁺	L-Isoleucine*	Amino acids and derivatives	Amino acids and derivatives	73-32-5	A	7.87E+05	1.12E+06	3.85E+06
	mws0227	132.1	86.2	131.095	[M+H] ⁺	L-Leucine*	Amino acids and derivatives	Amino acids and derivatives	61-90-5	A	8.03E+05	1.15E+06	3.76E+06
	mws0001	133.06	74	132.054	[M+H] ⁺	L-Asparagine	Amino acids and derivatives	Amino acids and derivatives	70-47-3	A	1.30E+05	3.10E+05	1.40E+06
	pme2527	133	116	132.09	[M+H] ⁺	L-Ornithine	Amino acids and derivatives	Amino acids and derivatives	70-26-8	A	9.00E+03	2.10E+04	2.22E+04
	mws0219	132.03	88	133.038	[M-H] ⁻	L-Aspartic Acid	Amino acids and derivatives	Amino acids and derivatives	56-84-8	A	2.16E+06	3.13E+06	1.13E+07
	pme0026	147.11	84	146.106	[M+H] ⁺	L-Lysine	Amino acids and derivatives	Amino acids and derivatives	56-87-1	A	1.23E+06	6.17E+06	1.16E+07
	pme0014	148.06	84	147.053	[M+H] ⁺	L-Glutamic acid	Amino acids and derivatives	Amino acids and derivatives	56-86-0	A	1.44E+07	1.36E+07	1.14E+07
	mws0254	156.08	110	155.069	[M+H] ⁺	L-Histidine	Amino acids and derivatives	Amino acids and derivatives	71-00-1	A	1.28E+05	3.85E+05	1.62E+06
	pme0021	166.09	120.08	165.07	[M+H] ⁺	L-Phenylalanine	Amino acids and derivatives	Amino acids and derivatives	63-91-2	A	6.98E+06	3.42E+06	1.53E+07
	pme0008	176.1	113	175.096	[M+H] ⁺	L-Citrulline	Amino acids and derivatives	Amino acids and derivatives	372-75-8	B	5.31E+04	1.99E+05	7.23E+05
	mws0250	182.08	136.1	181.074	[M+H] ⁺	L-Tyrosine	Amino acids and derivatives	Amino acids and derivatives	60-18-4	A	9.44E+06	7.66E+06	1.95E+07
	mws0282	203.08	116.05	204.09	[M-H] ⁻	L-Tryptophan	Amino acids and derivatives	Amino acids and derivatives	73-22-3	A	1.19E+06	8.75E+05	9.75E+06
	pme0193	147.08	84	146.069	[M+H] ⁺	L-Glutamine	Amino acids and derivatives	Amino acids and derivatives	56-85-9	A	1.10E+06	5.48E+06	1.06E+07
	pmb0863	492.31	184.07	491.301	[M+H] ⁺	LysoPC 16:2	Lipids	LPC	-	A	9.00E+00	2.21E+05	1.53E+05
	Lmhp008763	452.28	311.26	451.27	[M+H] ⁺	LysoPE 16:1	Lipids	LPE	-	A	1.96E+06	4.12E+04	1.84E+04
	mws0119	227.2	227.2	228.209	[M-H] ⁻	Myristic Acid	Lipids	Free fatty acids	544-63-8	A	9.00E+06	9.90E+06	4.48E+06
	pmn001610	307.26	307.3	308.272	[M-H] ⁻	Eicosadienoic acid	Lipids	Free fatty acids	5598-38-9	B	1.37E+05	7.84E+04	6.12E+04
	Lmbn005662	295.23	171.1	296.235	[M-H] ⁻	9(10)-EpOME;(9R,10S)-(12Z)-9,10-Epoxyoctadecenoic acid*	Lipids	Free fatty acids	16833-56-0	A	3.70E+04	2.13E+04	9.49E+03
	Zmyn004548	291.2	235.17	292.204	[M-H] ⁻	12-Oxo-phytodienoic acid	Lipids	Free fatty acids	85551-10-6	B	2.93E+04	1.38E+04	6.49E+03
Nucleotides and derivatives	MA10012327	300.29	60.04	299.282	[M+H] ⁺	D-Sphingosine	Lipids	Sphingolipids	123-78-4	B	2.75E+04	2.24E+04	2.64E+03
	mws0367	277.22	277.22	278.225	[M-H] ⁻	α -Linolenic Acid*	Lipids	Free fatty acids	463-40-1	A	3.64E+06	4.26E+06	3.63E+06
	mws0847	150.08	133	149.07	[M+H] ⁺	1-Methyladenine	Nucleotides and derivatives	Nucleotides and derivatives	5142-22-3	A	1.13E+05	1.40E+05	5.91E+05
	mws0255	112.05	95	111.043	[M+H] ⁺	Cytosine	Nucleotides and derivatives	Nucleotides and derivatives	71-30-7	A	3.09E+05	2.11E+05	9.31E+04
	pme0257	111.02	80	112.027	[M-H] ⁻	Uracil	Nucleotides and derivatives	Nucleotides and derivatives	66-22-8	A	1.70E+05	9.29E+04	9.84E+04
	pme0040	136.06	119	135.054	[M+H] ⁺	Adenine	Nucleotides and derivatives	Nucleotides and derivatives	73-24-5	A	2.19E+06	9.17E+05	3.21E+05
	pme0183	152.06	135	151.049	[M+H] ⁺	Isoguanine	Nucleotides and derivatives	Nucleotides and derivatives	3373-53-3	A	1.11E+05	1.11E+05	5.25E+05

Vitamin	pme1109	152.0 6	135	151.049	[M+H] ⁺	Guanine	Nucleotides and derivatives	Nucleotides and derivatives	73-40-5	A	6.87E+05	3.43E+04	4.40E+04
	pme0264	243.1	127	242.09	[M+H] ⁺	Thymidine	Nucleotides and derivatives	Nucleotides and derivatives	50-89-5	A	3.10E+05	9.85E+04	6.18E+04
	pme3732	244.0 9	112	243.086	[M+H] ⁺	Cytidine	Nucleotides and derivatives	Nucleotides and derivatives	65-46-3	A	1.70E+06	1.84E+06	5.83E+05
	pme0230	268.1	136.0 6	267.097	[M+H] ⁺	Adenosine	Nucleotides and derivatives	Nucleotides and derivatives	58-61-7	A	1.13E+06	1.41E+06	2.45E+05
	pme1184	268.1	152	267.097	[M+H] ⁺	2'-Deoxyguanosine	Nucleotides and derivatives	Nucleotides and derivatives	961-07-9	A	7.86E+05	1.18E+05	3.64E+04
	pme1178	284.1	152	283.092	[M+H] ⁺	Guanosine	Nucleotides and derivatives	Nucleotides and derivatives	118-00-3	A	6.29E+06	3.61E+06	1.60E+06
	mws0668	283.0 7	151	284.076	[M-H] ⁻	Xanthosine	Nucleotides and derivatives	Nucleotides and derivatives	146-80-5	A	1.92E+06	6.25E+06	5.67E+05
	mws0133	123.0 6	80.05	122.048	[M+H] ⁺	Nicotinamide	Others	Vitamin	98-92-0	B	1.88E+06	2.93E+05	1.61E+05
	pme0490	124.0 4	78	123.032	[M+H] ⁺	Vitamin B3	Others	Vitamin	59-67-6	B	8.77E+05	4.79E+05	3.41E+05
	pme1383	170.0 8	134.1	169.074	[M+H] ⁺	Pyridoxine	Others	Vitamin	65-23-6	B	1.80E+05	1.62E+05	2.95E+04
Phenolic acids	Hmfn000531	175.0 2	87.01	176.032	[M-H] ⁻	Vitamin C	Others	Vitamin	50-81-7	A	1.70E+04	3.26E+06	3.37E+06
	mws0232	377.1 5	243.0 9	376.138	[M+H] ⁺	Vitamin B2	Others	Vitamin	83-88-5	A	5.39E+05	4.76E+04	5.52E+04
	pme1014	445.3	341.3	444.303	[M+H] ⁺	Vitamin K2	Others	Vitamin	11032-49-8	B	2.64E+05	6.12E+04	7.23E+04
	pmf0096	88.99	70.9	89.995	[M-H] ⁻	Oxalic acid	Phenolic acids	Phenolic acids	144-62-7	B	3.06E+04	6.90E+04	4.00E+03
	Lmbn001930	121.0 3	77.04	122.037	[M-H] ⁻	2-Hydroxybenzaldehyde (Salicylaldehyde)	Phenolic acids	Phenolic acids	90-02-8	B	1.25E+05	2.18E+04	2.26E+04
	mws0628	121.0 3	92	122.037	[M-H] ⁻	4-Hydroxybenzaldehyde	Phenolic acids	Phenolic acids	123-08-0	A	8.08E+05	6.72E+04	5.42E+04
	Hmbn002174	135.0 5	120.0 2	136.053	[M-H] ⁻	4-Hydroxyacetophenone	Phenolic acids	Phenolic acids	99-93-4	A	1.80E+04	1.27E+05	1.52E+04
	mws1078	138.0 5	92.1	137.048	[M+H] ⁺	Anthranilic Acid	Phenolic acids	Phenolic acids	118-92-3	B	9.67E+04	3.43E+04	1.46E+04
	Hmgn001653	137.0 2	93.04	138.032	[M-H] ⁻	Protocatechualdehyde	Phenolic acids	Phenolic acids	139-85-5	B	4.62E+06	1.24E+05	9.39E+04
	mws0749	137.0 2	93	138.032	[M-H] ⁻	4-Hydroxybenzoic acid	Phenolic acids	Phenolic acids	99-96-7	A	6.10E+06	1.61E+05	1.08E+05
	mws2213	147.0 5	77.01	148.052	[M-H] ⁻	Cinnamic acid	Phenolic acids	Phenolic acids	140-10-3	B	2.82E+05	1.47E+04	9.00E+00
	mws0458	151.0 4	136	152.047	[M-H] ⁻	Vanillin	Phenolic acids	Phenolic acids	121-33-5	B	6.66E+06	1.92E+05	1.59E+05
	pme1439	165.0 5	119	164.047	[M+H] ⁺	p-Coumaric acid	Phenolic acids	Phenolic acids	501-98-4	B	2.92E+04	4.76E+04	2.91E+04
	pmb0142	165.1	95.2	164.047	[M+H] ⁺	Caffeic aldehyde	Phenolic acids	Phenolic acids	141632-15-7	B	3.36E+04	2.00E+04	3.54E+04
	pme3083	164.0 4	120	165.043	[M-H] ⁻	2-(Formylamino)benzoic acid	Phenolic acids	Phenolic acids	3342-77-6	B	6.88E+04	4.78E+04	1.20E+04
	NK10253223	168.0 6	94.06	167.058	[M+H] ⁺	2-Amino-3-methoxybenzoic acid	Phenolic acids	Phenolic acids	3177-80-8	B	9.90E+04	5.93E+04	2.95E+04
	mws0009	179.0 7	91	178.063	[M+H] ⁺	Coniferaldehyde	Phenolic acids	Phenolic acids	20649-42-7	B	1.43E+05	2.97E+04	9.16E+03

Flavonoids	mws2212	179.0 3	135.0 5	180.042	[M-H]-	Caffeic acid	Phenolic acids	Phenolic acids	331-39-5	A	1.32E+ 07	2.90E+ 05	1.16E+ 05
	mws0093	179.0 7	146	180.079	[M-H]-	Coniferyl alcohol	Phenolic acids	Phenolic acids	458-35-5	A	4.16E+ 05	5.68E+ 05	5.30E+ 05
	mws0014	193.0 5	134.0 1	194.058	[M-H]-	Ferulic acid	Phenolic acids	Phenolic acids	537-98-4	A	6.86E+ 06	1.29E+ 06	1.01E+ 06
	pmb2497	197	153	198.053	[M-H]-	4-Hydroxy-3-methoxymandelate	Phenolic acids	Phenolic acids	55-10-7	B	8.30E+ 04	4.96E+ 04	1.09E+ 05
	pme3472	271.0 9	107.6	272.09	[M-H]-	Arbutin	Phenolic acids	Phenolic acids	497-76-7	B	7.94E+ 05	8.91E+ 03	7.14E+ 03
	pmb0751	321.1	147.3	320.09	[M+H]+	Trans-5-O-(p-Coumaroyl)shikimate	Phenolic acids	Phenolic acids	-	B	7.03E+ 04	1.39E+ 04	9.00E+ 00
	pmb3074	337.0 9	191.0 5	338.1	[M-H]-	5-O-p-Coumaroylquinic acid	Phenolic acids	Phenolic acids	1899-30-5	B	5.81E+ 05	2.01E+ 05	3.56E+ 04
	mws0906	341.1 2	179	342.131	[M-H]-	Coniferin	Phenolic acids	Phenolic acids	531-29-3	B	2.45E+ 05	2.51E+ 05	9.00E+ 00
	mws0178	353.0 9	191.0 1	354.095	[M-H]-	Chlorogenic acid (3-O-Caffeoylquinic acid)	Phenolic acids	Phenolic acids	327-97-9	A	2.21E+ 07	2.66E+ 06	1.20E+ 06
	HJN003	385.1 1	223.0 6	386.122	[M-H]-	1-O-Sinapoyl-D-glucose	Phenolic acids	Phenolic acids	-	B	3.40E+ 04	5.99E+ 03	1.51E+ 04
	mws0918	283.0 6	268	284.068	[M-H]-	Prunetin (5,4'-Dihydroxy-7-methoxyisoflavone)	Flavonoids	Isoflavones	552-59-0	A	3.77E+ 05	2.04E+ 04	1.03E+ 05
	pme0088	285.0 4	151	286.048	[M-H]-	Luteolin (5,7,3',4'-Tetrahydroxyflavone)	Flavonoids	Flavonoid	491-70-3	B	1.29E+ 04	7.52E+ 02	5.36E+ 03
	mws0054	289.0 7	245	290.079	[M-H]-	Catechin	Flavonoids	Flavanols	154-23-4	B	4.18E+ 04	4.10E+ 05	1.16E+ 04
	pmp00112	301.0 7	286.0 8	300.063	[M+H]+	Chrysoeriol	Flavonoids	Flavonoid	491-71-4	B	6.49E+ 03	6.45E+ 03	6.07E+ 03
	mws0045	449.1 1	303.0 5	448.101	[M+H]+	Quercetin-3-O-rhamnoside(Quercitrin)	Flavonoids	Flavonols	522-12-3	B	1.54E+ 04	2.29E+ 04	8.54E+ 04
	mws2209	449.1 1	287.0 6	448.101	[M+H]+	Kaempferol-3-O-glucoside (Astragalin)	Flavonoids	Flavonols	480-10-4	B	1.77E+ 04	3.77E+ 04	1.60E+ 05
	pme2459	449.1 1	287.2	448.101	[M+H]+	Luteolin-7-O-glucoside (Cynaroside)	Flavonoids	Flavonoid	5373-11-5	A	9.56E+ 05	2.83E+ 04	1.78E+ 05
	mws0091	463.0 9	300.0 3	464.095	[M-H]-	Quercetin-3-O-glucoside (Isoquercitrin)*	Flavonoids	Flavonols	482-35-9	B	1.39E+ 04	4.94E+ 04	1.80E+ 05
	mws0059	609.1 5	301	610.153	[M-H]-	Quercetin-3-O-rutinoside (Rutin)*	Flavonoids	Flavonols	153-18-4	B	1.89E+ 04	3.93E+ 03	4.57E+ 03
Alkaloids	pmb0782	86.1	69.2	85.089	[M+H]+	Piperidine	Alkaloids	Alkaloids	110-89-4	B	3.22E+ 06	4.31E+ 06	1.47E+ 07
	pme2292	89.11	72.08	88.1	[M+H]+	Putrescine	Alkaloids	Phenolamine	110-60-1	B	3.03E+ 05	1.37E+ 06	7.20E+ 05
	pme1841	103.1 2	86.1	102.116	[M+H]+	Cadaverine	Alkaloids	Phenolamine	462-94-2	B	6.60E+ 04	1.50E+ 04	3.10E+ 04
	pmb1096	118.0 7	91	117.058	[M+H]+	Indole	Alkaloids	Plumerane	120-72-9	B	5.58E+ 03	4.10E+ 03	4.85E+ 04
	mws0191	118.0 9	59	117.079	[M+H]+	Betaine	Alkaloids	Alkaloids	107-43-7	B	1.09E+ 05	1.13E+ 05	2.75E+ 05
	pma3649	132.1	86.1	131.058	[M+H]+	5-Aminolevulinate	Alkaloids	Alkaloids	106-60-5	B	1.10E+ 05	2.14E+ 05	6.70E+ 05
	mws0017	146.1 7	72.2	145.158	[M+H]+	Spermidine	Alkaloids	Phenolamine	124-20-9	B	1.30E+ 06	2.27E+ 05	3.16E+ 05
	pme1691	147.1 3	87.2	146.118	[M+H]+	Acetylcholine	Alkaloids	Alkaloids	60-31-1	B	5.07E+ 05	1.94E+ 05	1.75E+ 05

	pmb0819	157	130	156.069	[M+H] ⁺	3-Indoleacetonitrile	Alkaloids	Plumerane	771-51-7	B	1.64E+04	2.02E+04	1.38E+05
	mws1346	162.08	98	161.069	[M+H] ⁺	DL-2-Aminoadipic acid	Alkaloids	Alkaloids	542-32-5	B	8.90E+05	3.05E+05	2.39E+05
	pme1651	176.1	130.1	175.063	[M+H] ⁺	Indole 3-acetic acid (IAA)	Alkaloids	Plumerane	87-51-4	B	4.87E+05	9.23E+03	3.51E+03
	pmb0818	206.1	147.5	205.074	[M+H] ⁺	Methoxyindoleacetic acid	Alkaloids	Plumerane	3471-31-6	B	4.07E+04	2.77E+04	3.13E+05
	Lmqn000780	606.08	384.98	607.082	[M-H] ⁻	Uridine 5'-diphospho-N-acetylglucosamine	Alkaloids	Alkaloids	528-04-1	B	2.35E+04	2.56E+04	5.32E+04
	mws0987	161.06	115	160.052	[M+H] ⁺	6-MethylCoumarin	Lignans and Coumarins	Coumarins	92-48-8	B	2.18E+04	9.17E+03	1.10E+04
	Hmjp002337	193.04	133.03	192.033	[M+H] ⁺	Isoscopoletin (6-Hydroxy-7-Methoxycoumarin)	Lignans and Coumarins	Coumarins	776-86-3	B	7.91E+04	3.98E+04	9.00E+00
	pmp000284	223.06	208.04	222.053	[M+H] ⁺	Fraxidin (8-Hydroxy-6,7-dimethoxycoumarin)*	Lignans and Coumarins	Coumarins	525-21-3	B	6.05E+04	1.08E+04	1.97E+03
	Cmpp008880	245.12	189.06	244.11	[M+H] ⁺	Suberosin	Lignans and Coumarins	Coumarins	581-31-7	B	2.90E+04	7.87E+03	1.98E+03
	Cmpp010709	299.16	163.04	298.157	[M+H] ⁺	Aurapten	Lignans and Coumarins	Coumarins	495-02-3	B	8.05E+03	6.47E+03	9.38E+03
Lignans and Coumarins	Cmpp011038	339.16	203.03	338.152	[M+H] ⁺	Bergamottin	Lignans and Coumarins	Coumarins	7380-40-7	B	6.33E+03	4.23E+03	5.36E+03
	mws4108	353.14	189.1	352.131	[M+H] ⁺	1-Methoxyphaseollin	Lignans and Coumarins	Coumarins	157226-48-7	B	9.00E+00	5.66E+03	2.71E+03
	mws1077	355.1	193.05	354.095	[M+H] ⁺	Scopoletin-7-O-glucoside (Scopolin)	Lignans and Coumarins	Coumarins	531-44-2	B	1.64E+06	6.60E+05	8.59E+04
	mws0097	357.13	151	358.142	[M-H] ⁻	Pinoresinol*	Lignans and Coumarins	Lignans	487-36-5	B	3.51E+04	1.02E+04	5.06E+03
	Lmdn004267	357.13	151.04	358.142	[M-H] ⁻	Epipinoresinol*	Lignans and Coumarins	Lignans	24404-50-0	B	3.09E+04	6.22E+03	3.16E+03
	Lmbn002160	373.13	343.12	374.137	[M-H] ⁻	8-Hydroxypinoresinol	Lignans and Coumarins	Lignans	81426-17-7	B	4.23E+05	1.22E+05	8.98E+04
Tannins	Lmfn000604	331.07	169.01	332.074	[M-H] ⁻	6-O-Galloyl-D-glucose	Tannins	Tannin	13186-19-1	B	5.12E+04	3.51E+04	5.19E+04
	pmn001518	331.07	169.01	332.074	[M-H] ⁻	1-O-Galloyl-D-glucose	Tannins	Tannin	58511-73-2	B	7.96E+04	3.44E+04	7.77E+04
	Hmln000659	331.07	169.01	332.075	[M-H] ⁻	3-O-Galloyl-D-glucose	Tannins	Tannin	-	B	5.20E+04	3.79E+04	4.85E+04
Triterpene	Lmzn006284	471.35	471.35	472.355	[M-H] ⁻	2 α -Hydroxyursolic acid	Terpenoids	Triterpene	-	B	1.42E+04	1.98E+04	2.73E+04
	Lmmn004145	675.41	397.14	679.419	[M-H] ⁻	3-O-(2-O-Acetyl-glucosyl)oleanolic acid	Terpenoids	Triterpene	-	B	4.06E+04	1.50E+05	5.52E+04
Proanthocyanidins	pme0434	577.14	407.1	578.142	[M-H] ⁻	Procyanidin B2	Tannins	Proanthocyanidins	29106-49-8	B	3.25E+03	9.00E+00	1.19E+04
Stilbene	pmn001399	405.12	243.1	406.126	[M-H] ⁻	2,4,6,4'-Tetrahydroxy-stilbene-2-O-glucoside	Others	Stilbene	-	B	5.05E+04	1.40E+04	4.78E+04