

# Comprehensive Metabolite Profiling in Genetic Resources of Garlic (*Allium sativum* L.) Collected from Different Geographical Regions

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**Supplementary Table S1.** Total saponin and fructan contents in the investigated garlic accessions.

World Collection No.	Sample name	Saponin (mg · g <sup>-1</sup> DW)*	Fructan (g · 100g <sup>-1</sup> FW)
AsWC146	JPN37	18.00	18.52
AsWC147	JPN39	3.36	18.12
AsWC148	JPN40	12.81	19.48
AsWC149	TWN45	13.49	18.22
AsWC150	CHN54	8.05	17.62
AsWC151	EGY55	4.27	16.41
AsWC154	JPN65	7.82	18.91
AsWC158	PER137	9.48	14.47
AsWC159	CHN180	10.67	18.69
AsWC162	GRE307	17.55	18.36
AsWC169	EGY489	32.18	12.16
AsWC173	CHN524	-	19.18**
AsWC175	TUR542	3.38	14.91**
AsWC177	GER556	9.83	10.93
AsWC181	F115	18.21	14.19
AsWC183	F138	17.21	13.97
AsWC186	F189	6.86	2.58
AsWC189	F1-200-34	17.53	10.47
AsWC193	Fs407	9.60	23.00
AsWC195	Fs414	10.10	10.24
AsWC196	Fs422	12.73	11.33
AsWC198	SANBARTOROME (Gatur)	23.68	15.96
AsWC201	SYR_No.5	29.82	-
AsWC202	IND-IIT	7.12	10.36
AsWC205	VNM_MaiDinh	17.71	10.47
AsWC208	THA67-4	-	-
AsWC209	THA16-5	-	11.08
AsWC214	JPN_Taishu-san	30.41	11.97
AsWC224	SHA_Shanghi	-	7.30
AsWC226	JPN_Kikai-onodu	24.96	-
	Mean	14.49	14.19
	Standaed Deviation	8.29	4.63
	Standard Error	1.63	0.93

-: No data.

\*The data of saponin contents were derived from Table 5 of the doctoral thesis (51). \*\*The fructan contents of the growth results at Yamaguchi in 2011 for two accessions, namely CHN524 and TUR542 were obtained from Figure 17 of the doctrol thesis (51).

**Supplementary Table S2.** List of normalized signal intensities of the metabolites identified in 30 garlic accessions

ID	Annotation	JPN37	JPN39	JPN40	TWN45	CHN54	EGY55	JPN65	PER13 7
X00004	1-Amino-1-cyclopentanecarboxylic acid	5.11	4.51	9.61	6.02	8.38	7.18	4.55	5.89
X00010	Citric acid,Anhydrous	2.57	2.30	1.33	2.27	4.24	2.94	3.25	0.71
X00039	Adenine	0.69	0.59	0.54	0.85	0.73	1.18	1.21	0.54
X00049	Glycine	0.15	0.09	0.32	0.20	0.19	0.36	0.24	0.19
X00054	L-(-)-Phenylalanine	1.17	1.14	1.20	1.02	0.98	2.27	3.40	2.50
X00055	L-Tryptophane	2.94	0.64	0.79	1.38	2.39	0.89	2.20	0.63
X00056	L-Tyrosine	0.31	0.22	0.32	0.49	0.65	0.40	0.94	0.30
X00060	Sucrose	7.57	5.77	5.00	5.39	4.60	6.63	5.31	5.37
X00095	Methylmalonic acid	0.42	0.49	0.34	0.40	0.40	0.44	0.33	0.35
X00099	Pyridoxamine dihydrochloride	0.04	0.05	0.10	0.05	0.06	0.10	0.08	0.07
X00187	Cystathionine	0.02	0.01	0.02	0.01	0.01	0.02	0.02	0.02
X00188	Cytidine,cell culture tested	1.42	0.92	1.36	1.32	1.42	2.99	4.01	0.76
X00212	DL-2,3-Diaminopropionic acid monohydrochloride	0.17	0.14	0.11	0.11	0.20	0.14	0.11	0.04
X00218	DL-threo-beta-Methylaspartic acid	0.12	0.09	0.07	0.10	0.10	0.10	0.05	0.06
X00241	Guanosine	0.20	0.33	0.25	0.27	0.17	0.43	0.20	0.20
X00256	Inosine	0.10	0.25	0.12	0.13	0.07	0.24	0.08	0.06
X00267	L-Asparagine	2.55	1.46	3.99	1.93	4.13	3.06	3.14	4.70
X00268	L-Aspartic acid	5.93	4.91	5.23	4.67	7.65	3.31	3.79	4.80
X00270	L-Cystine	0.05	0.07	0.04	0.10	0.04	0.10	0.05	0.06
X00272	L-Glutamic acid	39.38	38.09	47.04	50.36	56.08	54.88	37.35	35.72
X00273	L-Glutamine	22.26	17.12	51.20	20.34	33.05	33.04	23.88	32.13
X00285	L-Ornithine monohydrochloride	0.53	0.26	0.75	0.44	0.98	0.73	0.70	0.98
X00286	L-Proline	14.70	5.61	17.01	9.37	7.17	17.40	18.81	9.62
X00287	L-Pyroglutamic acid	5.55	4.93	10.94	6.92	10.31	7.73	4.59	6.58
X00288	L-Serine	6.95	4.56	9.66	4.76	6.39	10.41	9.83	7.57
X00338	S-Carboxymethyl-L-cysteine	0.18	0.14	0.19	0.10	0.19	0.12	0.17	0.15
X00344	Succinic acid	0.39	0.49	0.34	0.40	0.46	0.42	0.33	0.35
X00364	Tyramine	0.52	0.41	0.47	0.41	0.76	1.58	0.88	0.85
X00372	Uridine-5'-monophosphate	0.04	0.03	0.03	0.02	0.06	0.03	0.03	0.03
X00379	alpha-Lactose monohydrate	0.64	0.56	0.47	0.50	0.43	0.65	0.46	0.48
X00389	gamma-Amino-n-butyric acid	4.07	3.21	2.27	2.56	4.83	3.26	2.45	1.32
X00392	6-Aminohexanoic acid	0.72	0.36	0.48	0.64	0.96	0.58	1.40	0.47
X00416	Keracyanin Chloride	4.82	2.17	3.36	2.32	1.87	4.82	0.75	2.33
X00419	Isorhamnetin-3-O-glucoside	3.00	1.04	1.06	4.42	1.55	2.31	7.34	2.19
X00422	Kaempferol-3-O-glucoside	10.16	5.34	12.19	11.82	10.26	14.63	14.67	9.57
X00432	Hyperoside	1.69	0.56	0.80	2.08	0.65	1.70	5.25	1.39
X00477	O-Acetyl-L-serine hydrochloride	0.51	0.47	0.42	0.44	0.43	0.63	0.44	0.48
X00502	L-Saccharopine	0.19	0.16	0.23	0.31	0.39	0.26	0.42	0.18
X00675	5'-Deoxy-5'-Methylthioadenosine	2.42	1.36	2.38	1.56	2.06	2.60	2.16	1.45
X00695	L-allo-threonine	2.61	1.82	2.62	2.35	3.11	2.61	2.68	2.15
X00755	5-Aminovaleric acid	2.04	1.80	2.39	2.27	3.94	2.44	3.57	2.28

X00797	L-Threonic acid hemicalciums alt	0.86	0.77	0.48	0.84	0.81	0.92	0.57	0.46
X00849	Hesperidin	0.35	0.08	0.07	0.34	0.04	0.26	0.10	0.27
X00853	Luteolin-3',7-di-O-glucoside	4.86	3.43	6.31	6.02	4.79	7.41	8.45	4.27
X00854	Luteolin-4'-O-glucoside	21.85	11.97	28.01	26.62	22.11	33.31	34.37	21.09
X00860	Neohesperidin	0.81	0.23	0.17	0.73	0.08	0.48	0.21	0.51
X00865	Poncirin	0.22	0.06	0.16	0.06	0.04	0.17	0.05	0.11
X00906	Cysteinylglycine	1.20	1.32	1.34	0.87	0.86	1.01	1.08	1.13
X00907	DL-Homocysteine	0.02	0.01	0.02	0.03	0.06	0.05	0.01	0.01
X00921	Kaempferol-3-Rhamnoside-4"-Rhamnoside,-7-Rhamnoside	0.16	0.24	0.22	0.15	0.63	0.25	0.11	0.21
X00924	Kaempferol-3-Glucuronide	45.92	33.29	25.94	35.53	36.25	55.21	14.84	42.17
X00933	Quercetin-3-Glucuronide	21.62	15.22	7.39	26.53	6.82	31.34	9.64	19.18
X00943	alpha-Methyl-DL-histidine dihydrochloride	0.03	0.04	0.03	0.03	0.06	0.02	0.01	0.02
X00971	DL-5-Hydroxylysine hydrochloride	0.01	0.01	0.03	0.04	0.02	0.02	0.01	0.03
X00986	L-Anserine	0.04	0.05	0.03	0.04	0.04	0.04	0.04	0.04
X01016	Choline chloride	31.55	26.68	26.95	30.70	32.46	42.35	31.97	22.65
X01026	Trigonelline hydrochloride	4.35	1.75	0.77	3.45	3.28	2.29	1.30	1.45
X01097	DL-Pipecolic acid	3.56	2.65	6.95	3.33	5.93	5.16	3.27	4.91
X01098	Maleic acid	0.06	0.12	0.05	0.05	0.15	0.14	0.06	0.03
X01099	D-(+)-Raffinose pentahydrate	0.55	0.34	0.24	0.43	0.12	0.15	0.24	0.18
X01144	S-Methyl-L-cysteine	0.53	0.43	0.55	0.49	0.67	1.07	0.93	0.38
X01218	Petunidin-3-O-beta-glucopyranoside	3.61	3.80	1.29	5.76	2.25	3.26	5.22	3.04
X01219	Quercetin-3,4'-O-di-beta-glucopyranoside	0.44	0.10	0.10	0.52	0.06	0.29	0.76	0.30
X01220	Cyanidin-3-O-(2"-O-beta-xylopyranosyl-beta-glucopyranoside)	1.01	0.46	1.52	0.86	0.53	1.41	0.97	0.43
X01223	Delphinidin-3-O-(6"-O-alpha-rhamnopyranosyl-beta-glucopyranoside)	3.24	1.39	0.85	3.46	0.60	3.30	1.01	2.41
X01224	Delphinidin-3-O-(2"-O-beta-xylopyranosyl-beta-glucopyranoside)	0.27	0.23	0.09	0.45	0.11	0.26	0.46	0.27
X01225	Cyanidin-3-O-(2"-O-beta-xylopyranosyl-beta-glucopyranoside)-5-O-beta-glucopyranoside	0.38	0.36	0.27	0.16	0.35	0.22	0.24	0.17
X10002 4	L-Leucine, (Cell Culture Reagent, Crystalline)	0.97	0.43	0.63	1.02	1.26	0.76	1.85	0.60
X10002 5	L-Isoleucine	0.62	0.39	0.48	0.73	1.02	0.61	1.24	0.48
X10002 7	Methionine sulfoxide	0.13	0.09	0.18	0.19	0.16	0.17	0.54	0.17
X10003 9	Luteolin 7-O-glucuronide	46.15	34.22	26.66	37.68	37.66	48.10	14.28	43.67
X10004 3	2i_Leu_Ile	7.67	4.27	5.33	8.88	11.21	6.19	15.23	5.18
X10004 4	2i_Gln_Lys	41.16	30.46	93.40	37.58	64.14	59.30	44.86	57.94

X200004	3i_Isorhamnetin-3-O-rutinoside_Isorhamnetin-3-Glucoside-6"-Rhamnoside_Isorhamnetin-3-Galactoside-6"-Rhamnoside	8.87	3.30	1.54	10.25	1.67	5.15	2.15	5.88
X200007	2i_Cyanidin-3,5-di-O-glucoside chloride_Cyanidin-3-O-(2"-O-beta-glucopyranosyl-beta-glucopyranoside)	5.93	3.38	6.36	6.28	5.56	7.04	8.16	4.10
X200011	2i_Ideain chloride_Cyanidin-3-glucoside chloride	22.02	11.02	26.27	25.31	21.74	32.89	32.52	20.11
X200012	2i_Maritimein_luteolin-7-O-glucoside	17.44	11.36	21.65	20.76	17.69	26.82	26.38	16.43
X200017	2i_Syringetin-3-O-glucoside_Syringetin-3-O-galactoside	1.31	0.00	0.43	3.13	0.00	0.01	1.89	1.28
X200029	2i_alpha-D-Glucose-1-phosphate dipotassium salt dihydrate_alpha-D-Galactose-1-phosphate dipotassium salt pentahydrate	0.16	0.14	0.20	0.18	0.16	0.28	0.09	0.16
X200030	2i_D-Mannose-6-phosphate bariums salt hydrate_D-Mannose 6-phosphate mono sodiums salt	0.21	0.14	0.17	0.15	0.12	0.23	0.10	0.22
X200031	4i_D-Fructose-6-phosphate disodiums salt hydrate_D-Glucose-6-phosphate sodiums salt_alpha-D-(+)-mannose-1-phosphate sodiums salt hydrate_alpha-D-(+)Mannose 1-phosphate bis(cyclohexylammonium) salt	0.21	0.16	0.17	0.22	0.16	0.23	0.11	0.18
X200034	2i_D-(+)-Galactosamine hydrochloride_D-(+)-Glucosamine hydrochloride	0.03	0.03	0.03	0.05	0.05	0.08	0.08	0.06
X200042	2i_D-(+)-Cellobiose_Lactulose	0.72	0.58	0.52	0.54	0.43	0.73	0.53	0.55
X200043	6i_Melibiose hydrate_D-(+)-Turanose_Isomaltose_Gentiobiose_MelibiosePalatinose Monohydrate	4.76	3.70	3.16	3.60	2.99	4.26	3.31	3.26
X200047	4i_L(+)-Arginine HCl_N-alpha-Acetyl-L-ornithine_L-Citrulline	1.48	1.91	14.12	7.27	49.06	2.73	8.29	4.56
X200054	DL-Cysteine	0.02	0.02	0.02	0.01	0.02	0.01	0.02	0.02
X200055	2i_Nicotinamide_Niacinamide	0.51	0.33	0.40	0.39	0.46	0.93	0.62	0.28
X200057	2i_L-Alanine_Sarcosine	6.93	4.98	8.89	7.99	5.93	8.10	9.68	6.82
X200060	2i_L-Norvaline_L-Valine	3.36	2.92	4.09	3.52	6.17	4.06	6.10	3.89
X200061	3i_L-Threonine_alpha-Methyl-DL-serine_L-Homoserine	2.40	1.49	2.74	2.09	3.03	2.55	2.54	1.98
X200063	3i_L-2-Aminobutyric acid_N,N-Dimethylglycine hydrochloride_N-Methyl-DL-Alanine	5.91	5.41	5.24	5.69	6.32	8.06	6.22	4.33
X200068	DL-Malic acid	2.51	6.87	2.47	2.49	7.30	4.84	2.16	1.65

X20007 2	L-CarnitineHCl	0.03	0.01	0.02	0.04	0.05	0.02	0.02	0.04
X20007 3	DL-2-Amino adipic Acid	0.19	0.07	0.12	0.14	0.21	0.14	0.11	0.09
X20008 2	L-Lysine HCl	41.67	30.93	95.22	38.34	64.44	59.44	45.69	58.55
X20008 5	2i_L-Norleucine_D-Alloisoleucine	7.54	3.98	4.96	8.70	11.37	6.39	14.54	5.06
X20008 7	2i_Rutin_Quercetin-3-O-b-glucopyranosyl-7-O-a-rhamnopyranoside	2.26	0.57	0.58	2.02	0.23	1.33	0.58	1.43
X20008 9	2i_D-(+)-Melezitose monohydrate_1-Kestose	0.52	0.23	0.20	0.42	0.12	0.19	0.25	0.18
X26000 2	gamma-Glu-PRENC SO	1.27	0.30	1.46	0.66	0.87	1.04	0.93	0.56
X26000 6	MC SO	1.05	0.86	3.85	0.98	1.55	9.61	6.47	0.73
X26000 7	Alliin	39.55	18.79	37.95	22.57	27.00	30.74	31.45	30.19
<b>ID</b>	<b>Annotation</b>	<b>CHN180</b>	<b>GRE30 7</b>	<b>EGY48 9</b>	<b>CHN524</b>	<b>TUR542</b>	<b>GER556</b>	<b>F115</b>	<b>F138</b>
X00004	1-Amino-1-cyclopentanecarboxylic acid	4.02	5.80	4.80	4.10	6.87	3.52	3.51	4.00
X00010	Citric acid, Anhydrous	1.66	6.53	1.51	2.40	4.47	0.90	3.59	1.35
X00039	Adenine	1.42	1.61	0.44	0.68	0.99	0.85	0.84	0.95
X00049	Glycine	0.32	0.26	0.16	0.08	0.17	0.30	0.18	0.43
X00054	L-(-)-Phenylalanine	2.69	1.63	1.68	0.89	2.07	3.62	1.35	3.40
X00055	L-Tryptophane	3.97	2.32	0.28	0.47	1.15	4.00	0.50	2.13
X00056	L-Tyrosine	1.28	1.10	0.15	0.31	0.44	0.73	0.34	0.60
X00060	Sucrose	5.02	5.85	4.73	3.17	6.85	7.30	4.25	7.77
X00095	Methylmalonic acid	0.38	0.32	0.34	0.42	0.50	0.37	0.30	0.59
X00099	Pyridoxamine dihydrochloride	0.07	0.12	0.06	0.07	0.05	0.06	0.16	0.09
X00187	Cystathionine	0.01	0.01	0.01	0.02	0.01	0.01	0.01	0.01
X00188	Cytidine, cell culture tested	1.89	6.30	0.85	0.90	1.85	1.36	1.06	1.30
X00212	DL-2,3-Diaminopropionic acid monohydrochloride	0.05	0.25	0.08	0.16	0.16	0.21	0.12	0.25
X00218	DL-threo-beta-Methylaspartic acid	0.05	0.10	0.06	0.06	0.11	0.02	0.05	0.06
X00241	Guanosine	0.31	0.26	0.50	0.24	0.27	0.24	0.18	0.32
X00256	Inosine	0.13	0.12	0.36	0.14	0.12	0.12	0.07	0.19
X00267	L-Asparagine	2.97	3.20	4.44	3.24	3.78	1.18	1.39	1.40
X00268	L-Aspartic acid	3.31	4.35	4.06	4.01	4.93	2.63	3.22	3.45
X00270	L-Cystine	0.04	0.07	0.05	0.02	0.04	0.14	0.02	0.12
X00272	L-Glutamic acid	37.38	32.97	34.47	25.38	42.93	28.49	24.15	39.71
X00273	L-Glutamine	27.07	28.12	22.30	27.41	23.18	15.97	16.45	20.39
X00285	L-Ornithine monohydrochloride	0.71	0.78	0.89	0.82	0.64	0.77	0.36	0.36
X00286	L-Proline	16.36	15.24	9.06	6.23	9.41	13.12	5.80	14.70
X00287	L-Pyroglutamic acid	4.35	6.23	5.30	4.64	7.19	3.72	3.65	4.40
X00288	L-Serine	6.16	7.16	7.32	5.23	8.53	3.08	3.18	7.03

X00338	S-Carboxymethyl-L-cysteine	0.14	0.08	0.13	0.10	0.14	0.12	0.08	0.10
X00344	Succinic acid	0.35	0.29	0.33	0.44	0.51	0.41	0.33	0.59
X00364	Tyramine	0.81	0.57	1.00	0.97	1.10	0.22	0.69	0.48
X00372	Uridine-5'-monophosphate	0.03	0.02	0.02	0.03	0.05	0.05	0.03	0.03
X00379	alpha-Lactose monohydrate	0.52	0.57	0.40	0.33	0.62	0.62	0.39	0.73
X00389	gamma-Amino-n-butyric acid	1.34	4.62	1.92	3.40	3.22	4.28	2.66	4.67
X00392	6-Aminoheptanoic acid	1.88	1.22	0.30	0.36	0.73	0.87	0.39	0.77
X00416	Keracyanin Chloride	0.87	3.99	3.60	2.33	4.10	2.08	1.59	3.48
X00419	Isorhamnetin-3-O-glucoside	8.30	16.75	0.84	3.28	3.34	1.88	0.86	1.14
X00422	Kaempferol-3-O-glucoside	18.00	21.91	6.01	7.43	17.11	10.43	4.08	6.45
X00432	Hyperoside	5.15	14.61	0.51	2.72	3.74	1.32	0.80	0.65
X00477	O-Acetyl-L-serine hydrochloride	0.47	0.41	0.52	0.43	0.69	0.22	0.43	0.40
X00502	L-Saccharopine	0.51	0.52	0.10	0.18	0.27	0.27	0.15	0.17
X00675	5'-Deoxy-5'-Methylthioadenosine	1.37	2.28	1.48	1.10	2.80	0.97	1.54	1.36
X00695	L-allo-threonine	2.84	2.58	1.93	1.41	2.28	2.17	1.14	2.18
X00755	5-Aminovaleric acid	4.24	3.54	1.82	1.43	2.23	2.63	1.59	3.20
X00797	L-Threonic acid hemicalcium salt	0.76	0.69	0.67	0.71	1.02	0.74	1.11	0.75
X00849	Hesperidin	0.17	0.36	0.20	0.31	0.40	0.02	0.13	0.08
X00853	Luteolin-3',7-di-O-glucoside	10.48	13.72	2.97	4.23	8.03	2.85	2.51	1.85
X00854	Luteolin-4'-O-glucoside	40.61	50.48	13.33	17.93	37.50	21.18	9.82	13.20
X00860	Neohesperidin	0.34	0.75	0.46	0.64	0.81	0.10	0.25	0.15
X00865	Poncirin	0.17	0.18	0.12	0.10	0.17	0.06	0.01	0.10
X00906	Cysteinylglycine	1.28	0.84	0.97	0.95	0.43	1.14	0.79	0.92
X00907	DL-Homocysteine	0.01	0.00	0.02	0.01	0.02	0.03	0.02	0.04
X00921	Kaempferol-3-Rhamnoside-4''-Rhamnoside,-7-Rhamnoside	0.12	0.09	0.17	0.15	0.20	0.09	0.22	0.19
X00924	Kaempferol-3-Glucuronide	15.10	33.19	44.22	35.21	53.75	29.40	53.39	52.81
X00933	Quercetin-3-Glucuronide	8.60	26.34	25.21	24.12	26.49	9.16	35.96	22.94
X00943	alpha-Methyl-DL-histidine dihydrochloride	0.03	0.01	0.02	0.02	0.03	0.01	0.01	0.02
X00971	DL-5-Hydroxylysine hydrochloride	0.02	0.02	0.01	0.02	0.02	0.01	0.00	0.00
X00986	L-Anserine	0.05	0.04	0.06	0.04	0.02	0.04	0.04	0.05
X01016	Choline chloride	28.90	36.84	28.60	21.19	39.10	21.83	28.85	29.45
X01026	Trigonelline hydrochloride	2.12	4.83	1.29	1.63	2.17	2.17	1.87	2.10
X01097	DL-Pipecolic acid	3.16	3.70	2.83	4.05	3.93	3.14	2.73	2.90
X01098	Maleic acid	0.07	0.08	0.05	0.04	0.10	0.03	0.11	0.07
X01099	D-(+)-Raffinose pentahydrate	0.24	0.37	0.14	0.24	0.38	1.50	0.19	0.57
X01144	S-Methyl-L-cysteine	0.90	1.28	0.38	0.55	0.66	0.63	0.65	0.75
X01218	Petunidin-3-O-beta-glucopyranoside	6.44	7.17	2.76	4.05	7.15	3.62	8.64	3.58
X01219	Quercetin-3,4'-O-di-beta-glucopyranoside	0.68	1.64	0.20	0.32	0.56	0.14	0.39	0.10
X01220	Cyanidin-3-O-(2''-O-beta-xylopyranosyl-beta-glucopyranoside)	1.29	2.09	0.35	0.49	1.24	0.94	0.36	0.38
X01223	Delphinidin-3-O-(6''-O-alpha-rhamnopyranosyl-beta-glucopyranoside)	1.27	4.52	3.23	4.04	4.23	0.77	2.36	1.66
X01224	Delphinidin-3-O-(2''-O-beta-xylopyranosyl-beta-glucopyranoside)	0.51	0.64	0.24	0.34	0.53	0.21	0.45	0.19

X01225	Cyanidin-3-O-(2"-O-beta-xylopyranosyl-beta-glucopyranoside)-5-O-beta-glucopyranoside	0.26	0.30	0.13	0.12	0.42	0.38	0.50	0.33
X100024	L-Leucine, (Cell Culture Reagent, Crystalline)	2.59	1.91	0.31	0.48	0.97	1.23	0.51	0.94
X100025	L-Isoleucine	1.83	1.29	0.28	0.39	0.69	0.88	0.40	0.79
X100027	Methionine sulfoxide	0.68	0.43	0.07	0.13	0.20	0.34	0.10	0.26
X100039	Luteolin 7-O-glucuronide	15.56	35.04	45.72	35.56	56.98	30.18	54.75	53.02
X100043	2i_Leu_Ile	21.96	15.49	2.95	4.08	8.43	10.28	4.36	8.48
X100044	2i_Gln_Lys	50.53	52.89	39.60	48.67	42.99	31.53	29.45	37.67
X200004	3i_Isorhamnetin-3-O-rutinoside_Isorhamnetin-3-Glucoside-6"-Rhamnoside_Isorhamnetin-3-Galactoside-6"-Rhamnoside	2.61	9.11	8.62	9.54	7.41	2.15	4.96	5.15
X200007	2i_Cyanidin-3,5-di-O-glucoside chloride_Cyanidin-3-O-(2"-O-beta-glucopyranosyl-beta-glucopyranoside)	10.84	14.47	3.21	4.09	8.17	3.05	2.60	1.79
X200011	2i_Ideain chloride_Cyanidin-3-glucoside chloride	38.64	47.69	12.19	17.05	36.64	21.24	10.21	8.95
X200012	2i_Maritimein_luteolin-7-O-glucoside	31.66	40.16	10.51	13.32	30.51	17.22	7.48	10.28
X200017	2i_Syringetin-3-O-glucoside_Syringetin-3-O-galactoside	1.17	2.22	1.37	1.86	2.70	0.11	0.17	0.06
X200029	2i_alpha-D-Glucose-1-phosphate dipotassium salt dihydrate_alpha-D-Galactose-1-phosphate dipotassium salt pentahydrate	0.22	0.08	0.21	0.13	0.22	0.09	0.10	0.11
X200030	2i_D-Mannose-6-phosphate bariums salt hydrate_D-Mannose 6-phosphate mono sodiums salt	0.26	0.08	0.16	0.23	0.21	0.03	0.09	0.11
X200031	4i_D-Fructose-6-phosphate disodiums salt hydrate_D-Glucose-6-phosphate sodiums salt_alpha-D-(+)-mannose-1-phosphate sodiums salt hydrate_alpha-D-(+)Mannose 1-phosphate bis(cyclohexylammonium) salt	0.23	0.08	0.16	0.26	0.20	0.08	0.14	0.11
X200034	2i_D-(+)-Galactosamine hydrochloride_D-(+)-Glucosamine hydrochloride	0.08	0.05	0.04	0.02	0.04	0.04	0.03	0.04
X200042	2i_D-(+)-Cellobiose_Lactulose	0.58	0.57	0.46	0.33	0.74	0.80	0.40	0.79
X200043	6i_Melibiose hydrate_D-(+)-Turanose_Isomaltose_Gentiobiose_MelibiosePalatinose Monohydrate	3.42	3.74	2.91	2.02	4.40	4.65	2.77	5.03
X200047	4i_L-(+)-Arginine HCl_N-alpha-Acetyl-L-ornithine_L-Citrulline	7.83	16.35	4.74	3.98	3.95	15.10	1.28	2.03



X200054	DL-Cysteine	0.02	0.01	0.01	0.01	0.04	0.02	0.01	0.03
X200055	2i_Nicotinamide_Niacinamide	0.50	0.84	0.36	0.36	0.61	0.30	0.48	0.44
X200057	2i_L-Alanine_Sarcosine	9.91	7.92	6.20	5.25	8.05	7.22	6.12	7.65
X200060	2i_L-Norvaline_L-Valine	6.79	5.48	2.94	2.30	3.43	4.23	2.78	5.41
X200061	3i_L-Threonine_alpha-Methyl-DL-serine_L-Homoserine	2.84	2.23	1.71	1.18	2.31	1.84	1.20	2.14
X200063	3i_L-2-Aminobutyric acid_N,N-Dimethylglycine hydrochloride_N-Methyl-DL-Alanine	5.84	7.14	5.84	4.27	7.66	4.26	5.84	5.69
X200068	DL-Malic acid	2.66	2.83	2.73	2.28	3.73	1.61	6.62	2.92
X200072	L-CarnitineHCl	0.03	0.01	0.03	0.03	0.02	0.02	0.03	0.03
X200073	DL-2-Aminoadipic Acid	0.11	0.08	0.08	0.06	0.12	0.09	0.05	0.08
X200082	L-Lysine HCl	51.60	53.53	40.00	48.73	43.84	31.71	29.25	37.78
X200085	2i_L-Norleucine_D-Alloisoleucine	21.32	15.74	2.90	3.75	7.40	10.61	4.19	8.07
X200087	2i_Rutin_Quercetin-3-O-b-glucopyranosyl-7-O-a-rhamnopyranoside	1.01	2.34	1.35	1.87	2.07	0.29	0.79	0.56
X200089	2i_D-(+)-Melezitose monohydrate_1-Kestose	0.20	0.39	0.16	0.20	0.36	1.52	0.13	0.54
X260002	gamma-Glu-PRENC SO	0.63	0.40	0.49	0.08	0.63	0.78	0.10	0.92
X260006	MCSO	1.11	1.17	2.35	2.02	4.08	13.60	9.99	14.04
X260007	Alliin	25.56	17.67	24.13	18.01	25.42	23.08	14.24	25.09
<b>ID</b>	<b>Annotation</b>	<b>F189</b>	<b>F1-200-34</b>	<b>Fs407</b>	<b>Fs414</b>	<b>Fs422</b>	<b>SAN BARTOROME (Gatur)</b>	<b>SYR_No. 5</b>	<b>IND-III</b>
X00004	1-Amino-1-cyclopentanecarboxylic acid	3.55	5.70	2.27	5.23	3.83	5.36	6.08	11.17
X00010	Citric acid,Anhydrous	1.29	3.03	1.71	4.15	2.41	3.71	0.41	3.92
X00039	Adenine	0.74	0.85	0.67	0.76	0.70	1.32	0.39	1.73
X00049	Glycine	0.56	0.61	0.28	0.14	0.08	0.24	0.13	0.48
X00054	L-(-)-Phenylalanine	6.59	5.15	6.36	2.42	1.37	2.71	1.46	2.55
X00055	L-Tryptophane	2.96	2.99	1.64	1.06	0.26	2.16	0.31	3.78
X00056	L-Tyrosine	0.87	0.83	0.53	0.41	0.21	0.79	0.20	1.38
X00060	Sucrose	7.42	7.56	7.08	5.22	2.92	5.60	3.84	8.37
X00095	Methylmalonic acid	0.28	0.59	0.38	0.49	0.40	0.36	0.29	0.33
X00099	Pyridoxamine dihydrochloride	0.12	0.13	0.06	0.08	0.04	0.18	0.11	0.11

X00187	Cystathionine	0.02	0.02	0.02	0.02	0.02	0.03	0.01	0.01
X00188	Cytidine,cell culture tested	1.54	3.25	1.07	1.99	0.88	3.57	0.81	5.07
X00212	DL-2,3-Diaminopropionic acid monohydrochloride	0.13	0.24	0.17	0.12	0.09	0.10	0.04	0.20
X00218	DL-threo-beta-Methylaspartic acid	0.05	0.08	0.04	0.04	0.06	0.06	0.05	0.10
X00241	Guanosine	0.13	0.52	0.30	0.45	0.24	0.34	0.30	0.66
X00256	Inosine	0.07	0.37	0.13	0.23	0.15	0.20	0.20	0.28
X00267	L-Asparagine	2.49	5.05	2.18	1.93	1.40	3.59	5.03	4.13
X00268	L-Aspartic acid	3.52	5.76	2.23	5.49	3.54	6.15	3.34	3.72
X00270	L-Cystine	0.07	0.15	0.08	0.10	0.02	0.02	0.06	0.11
X00272	L-Glutamic acid	33.72	37.63	25.13	36.44	22.13	42.17	32.92	49.66
X00273	L-Glutamine	36.63	37.43	20.66	27.27	15.08	36.21	38.37	57.37
X00285	L-Ornithine monohydrochloride	0.69	1.65	0.60	0.46	0.28	0.80	1.07	0.99
X00286	L-Proline	13.86	12.18	8.67	9.19	4.16	14.83	10.09	30.70
X00287	L-Pyroglutamic acid	3.89	7.59	2.52	5.80	3.97	5.64	7.00	12.58
X00288	L-Serine	6.70	5.77	4.11	6.16	2.76	9.24	5.02	7.02
X00338	S-Carboxymethyl-L-cysteine	0.09	0.16	0.09	0.16	0.09	0.14	0.07	0.12
X00344	Succinic acid	0.25	0.60	0.36	0.51	0.39	0.40	0.32	0.32
X00364	Tyramine	0.34	0.42	0.89	0.19	0.14	1.06	0.69	0.69
X00372	Uridine-5'-monophosphate	0.03	0.03	0.03	0.02	0.02	0.04	0.02	0.04
X00379	alpha-Lactose monohydrate	0.68	0.69	0.62	0.40	0.26	0.57	0.32	0.74
X00389	gamma-Amino-n-butyric acid	2.74	4.96	4.26	2.72	1.91	2.74	1.22	3.98
X00392	6-Aminoheptanoic acid	1.19	1.20	0.73	0.73	0.24	1.13	0.32	1.49
X00416	Keracyanin Chloride	2.55	3.01	2.01	3.54	1.22	2.41	1.59	1.71
X00419	Isorhamnetin-3-O-glucoside	2.15	1.28	1.12	1.14	1.30	7.62	0.50	2.85
X00422	Kaempferol-3-O-glucoside	10.68	6.46	6.22	10.37	13.94	16.41	8.18	26.77
X00432	Hyperoside	1.16	0.65	0.80	0.73	0.13	6.00	0.35	3.60
X00477	O-Acetyl-L-serine hydrochloride	0.36	0.33	0.33	0.53	0.52	0.41	0.38	0.44
X00502	L-Saccharopine	0.29	0.23	0.19	0.18	0.12	0.50	0.12	0.58
X00675	5'-Deoxy-5'-Methylthioadenosine	1.23	2.47	1.06	2.45	1.91	1.94	0.85	2.48
X00695	L-allo-threonine	2.42	3.04	1.82	2.35	0.83	2.96	1.79	3.58
X00755	5-Aminovaleric acid	3.95	3.69	3.20	2.66	1.09	3.62	1.64	4.14
X00797	L-Threonic acid hemicalciums salt	0.67	0.89	0.84	1.11	0.86	0.88	0.46	1.12
X00849	Hesperidin	0.04	0.05	0.16	0.12	0.06	0.18	0.04	0.13
X00853	Luteolin-3',7-di-O-glucoside	3.60	3.06	1.83	4.76	5.97	8.33	3.82	10.14
X00854	Luteolin-4'-O-glucoside	20.80	22.62	13.10	31.93	47.60	37.19	18.37	59.43
X00860	Neohesperidin	0.09	0.13	0.32	0.21	0.10	0.41	0.14	0.27
X00865	Poncirin	0.11	0.09	0.06	0.13	0.01	0.12	0.05	0.01
X00906	Cysteinylglycine	0.85	1.43	1.03	1.59	0.79	1.66	0.77	1.22
X00907	DL-Homocysteine	0.02	0.10	0.03	0.02	0.02	0.03	0.02	0.05
X00921	Kaempferol-3-Rhamnoside-4"-Rhamnoside,-7-Rhamnoside	0.19	0.13	0.12	0.25	0.23	0.17	0.11	0.42
X00924	Kaempferol-3-Glucuronide	45.52	43.00	32.21	69.91	27.64	34.28	17.59	57.96
X00933	Quercetin-3-Glucuronide	16.92	15.90	26.38	19.41	18.58	15.20	7.89	28.49
X00943	alpha-Methyl-DL-histidine dihydrochloride	0.02	0.04	0.01	0.02	0.02	0.03	0.02	0.02
X00971	DL-5-Hydroxylysine hydrochloride	0.02	0.01	0.01	0.01	0.04	0.02	0.01	0.02

X00986	L-Anserine	0.04	0.03	0.06	0.04	0.03	0.07	0.04	0.05
X01016	Choline chloride	26.02	32.47	23.21	37.13	28.95	31.15	19.33	41.05
X01026	Trigonelline hydrochloride	2.34	3.16	1.65	1.90	0.95	2.17	1.28	4.32
X01097	DL-Pipecolic acid	5.52	5.45	1.92	3.91	2.77	5.50	6.01	9.16
X01098	Maleic acid	0.03	0.09	0.06	0.11	0.06	0.07	0.05	0.11
X01099	D-(+)-Raffinose pentahydrate	0.68	0.53	0.80	0.31	0.20	0.25	0.07	0.53
X01144	S-Methyl-L-cysteine	0.65	1.13	0.70	0.69	0.60	0.82	0.52	1.20
X01218	Petunidin-3-O-beta-glucopyranoside	4.30	3.61	5.11	9.24	43.08	5.92	1.19	7.54
X01219	Quercetin-3,4'-O-di-beta-glucopyranoside	0.15	0.16	0.26	0.37	0.47	0.70	0.09	0.27
X01220	Cyanidin-3-O-(2"-O-beta-xylopyranosyl-beta-glucopyranoside)	0.61	0.84	0.29	1.06	1.50	0.97	0.74	2.43
X01223	Delphinidin-3-O-(6"-O-alpha-rhamnopyranosyl-beta-glucopyranoside)	1.00	1.12	2.60	1.77	1.48	2.44	0.67	2.04
X01224	Delphinidin-3-O-(2"-O-beta-xylopyranosyl-beta-glucopyranoside)	0.21	0.24	0.29	0.42	2.19	0.50	0.09	0.60
X01225	Cyanidin-3-O-(2"-O-beta-xylopyranosyl-beta-glucopyranoside)-5-O-beta-glucopyranoside	0.46	0.49	0.32	1.11	1.94	0.28	0.11	0.67
X10002 4	L-Leucine, (Cell Culture Reagent, Crystalline)	1.57	1.54	0.85	0.97	0.32	1.68	0.38	2.50
X10002 5	L-Isoleucine	1.21	1.13	0.63	0.65	0.22	1.15	0.29	1.46
X10002 7	Methionine sulfoxide	0.36	0.39	0.22	0.15	0.06	0.48	0.08	0.50
X10003 9	Luteolin 7-O-glucuronide	48.33	44.03	32.29	72.63	29.03	35.60	17.94	40.23
X10004 3	2i_Leu_Ile	13.33	13.10	7.59	8.17	2.59	14.31	3.40	19.75
X10004 4	2i_Gln_Lys	65.76	68.33	36.04	48.97	27.77	65.66	68.75	104.25
X20000 4	3i_Isorhamnetin-3-O-rutinoside_Isorhamnetin-3-Glucoside-6"-Rhamnoside_Isorhamnetin-3-Galactoside-6"-Rhamnoside	3.69	2.99	5.35	4.87	4.07	4.56	1.24	2.97
X20000 7	2i_Cyanidin-3,5-di-O-glucoside chloride_Cyanidin-3-O-(2"-O-beta-glucopyranosyl-beta-glucopyranoside)	3.51	3.72	1.75	4.81	6.15	8.26	3.82	10.01
X20001 1	2i_Ideain chloride_Cyanidin-3-glucoside chloride	19.28	21.09	11.34	23.35	45.84	35.69	16.95	56.95
X20001 2	2i_Maritimein_luteolin-7-O-glucoside	18.16	16.77	10.26	19.18	24.12	28.36	14.25	45.85
X20001 7	2i_Syringetin-3-O-glucoside_Syringetin-3-O-galactoside	0.07	0.22	0.21	0.09	0.19	1.71	0.01	0.01
X20002 9	2i_alpha-D-Glucose-1-phosphate dipotassium salt dihydrate_alpha-D-Galactose-1-phosphate dipotassium salt pentahydrate	0.06	0.10	0.09	0.14	0.09	0.22	0.14	0.15

X200030	2i_D-Mannose-6-phosphate barium salt hydrate_D-Mannose 6-phosphate mono sodium salt	0.11	0.07	0.12	0.12	0.03	0.21	0.10	0.14
X200031	4i_D-Fructose-6-phosphate disodium salt hydrate_D-Glucose-6-phosphate sodium salt_alpha-D-(+)-mannose-1-phosphate sodium salt hydrate_alpha-D-(+)Mannose 1-phosphate bis(cyclohexyl ammonium) salt	0.12	0.06	0.12	0.16	0.09	0.23	0.11	0.13
X200034	2i_D(+)-Galactosamine hydrochloride_D-(+)-Glucosamine hydrochloride	0.05	0.04	0.04	0.03	0.03	0.03	0.08	0.07
X200042	2i_D-(+)-Cellobiose_Lactulose	0.82	0.80	0.70	0.50	0.29	0.63	0.35	0.91
X200043	6i_Melibiose hydrate_D-(+)-Turanose_Isomaltose_Gentiobiose_Melibiose Palatinose Monohydrate	4.60	5.08	4.52	3.31	1.81	3.61	2.30	5.69
X200047	4i_L(+)-Arginine HCl_N-alpha-Acetyl-L-ornithine_L-Citrulline	6.80	48.19	2.24	5.54	2.17	7.08	12.71	9.95
X200054	DL-Cysteine	0.01	0.03	0.01	0.03	0.02	0.02	0.02	0.03
X200055	2i_Nicotinamide_Niacinamide	0.39	0.41	0.36	0.64	0.29	0.68	0.23	0.72
X200057	2i_L-Alanine_Sarcosine	7.00	9.80	7.16	5.48	6.59	7.02	5.78	11.16
X200060	2i_L-Norvaline_L-Valine	6.40	6.30	5.26	4.12	1.90	6.10	2.81	6.78
X200061	3i_L-Threonine_alpha-Methyl-DL-serine_L-Homoserine	2.41	3.03	1.53	2.14	0.86	2.70	1.66	3.57
X200063	3i_L-2-Aminobutyric acid_N,N-Dimethylglycine hydrochloride_N-Methyl-DL-Alanine	5.10	6.64	4.42	7.19	5.69	6.09	4.06	8.42
X200068	DL-Malic acid	2.28	3.52	3.54	5.68	2.76	3.04	1.93	4.38
X200072	L-Carnitine HCl	0.04	0.04	0.04	0.03	0.03	0.02	0.04	0.12
X200073	DL-2-Amino adipic Acid	0.07	0.09	0.03	0.05	0.02	0.09	0.06	0.16
X200082	L-Lysine HCl	65.05	68.31	36.62	49.73	27.37	67.50	68.74	105.35
X200085	2i_L-Norleucine_D-Alloisoleucine	12.93	11.58	7.29	8.13	2.62	13.74	3.22	20.06
X200087	2i_Rutin_Quercetin-3-O-beta-D-glucopyranosyl-7-O-alpha-D-rhamnopyranoside	0.36	0.42	0.92	0.66	0.47	1.22	0.38	0.77
X200089	2i_D-(+)-Melezitose monohydrate_1-Kestose	0.71	0.53	0.81	0.27	0.12	0.23	0.04	0.54
X260002	gamma-Glu-PRENC SO	0.77	1.61	0.99	0.85	0.10	0.39	0.36	0.53
X260006	MCSO	12.59	33.57	8.23	13.04	11.02	1.68	5.37	4.93

X260007	Alliin	24.48	44.98	21.42	36.37	13.21	30.51	17.57	25.60
<b>ID</b>	<b>Annotation</b>	VNM_Ma i Dinh	THA67- 4	THA 16- 5	JPN_Taishu -san	SHA_Shangh i	JPN_Kikai- onodu		
X00004	1-Amino-1-cyclopentanecarboxylic acid	3.88	9.58	7.55	4.75	9.32	3.72		
X00010	Citric acid,Anhydrous	2.25	0.88	1.50	2.86	1.42	1.10		
X00039	Adenine	1.00	1.12	1.27	1.19	0.59	0.89		
X00049	Glycine	0.16	0.36	0.34	0.21	0.60	0.22		
X00054	L-(-)-Phenylalanine	0.80	1.02	1.27	1.51	2.02	2.33		
X00055	L-Tryptophane	0.97	1.03	1.99	2.79	1.37	2.44		
X00056	L-Tyrosine	0.28	0.59	0.84	0.89	0.48	0.88		
X00060	Sucrose	6.55	5.51	6.02	5.81	7.22	5.91		
X00095	Methylmalonic acid	0.29	0.35	0.31	0.24	0.24	0.32		
X00099	Pyridoxamine dihydrochloride	0.04	0.10	0.09	0.05	0.12	0.07		
X00187	Cystathionine	0.02	0.01	0.01	0.00	0.02	0.01		
X00188	Cytidine,cell culture tested	1.14	1.71	2.03	2.75	1.63	2.14		
X00212	DL-2,3-Diaminopropionic acid monohydrochloride	0.25	0.11	0.17	0.15	0.11	0.08		
X00218	DL-threo-beta-Methylaspartic acid	0.10	0.08	0.09	0.05	0.10	0.06		
X00241	Guanosine	0.28	0.27	0.29	0.60	0.47	0.27		
X00256	Inosine	0.22	0.17	0.21	0.20	0.34	0.20		
X00267	L-Asparagine	0.69	4.19	3.06	1.18	5.98	1.29		
X00268	L-Aspartic acid	4.33	4.52	4.82	2.73	7.87	2.62		
X00270	L-Cystine	0.10	0.04	0.11	0.05	0.06	0.04		
X00272	L-Glutamic acid	54.10	50.96	54.48	37.97	49.32	35.05		
X00273	L-Glutamine	10.80	38.67	27.02	17.54	46.48	15.50		
X00285	L-Ornithine monohydrochloride	0.15	0.85	0.64	0.29	1.18	0.46		
X00286	L-Proline	6.65	11.78	15.06	13.03	16.95	11.23		
X00287	L-Pyroglutamic acid	3.90	10.61	7.91	5.05	9.87	3.93		
X00288	L-Serine	6.15	9.94	6.15	6.58	14.76	4.92		
X00338	S-Carboxymethyl-L-cysteine	0.16	0.06	0.10	0.06	0.20	0.09		
X00344	Succinic acid	0.35	0.34	0.39	0.28	0.23	0.30		
X00364	Tyramine	0.50	0.92	0.74	0.68	1.12	0.76		
X00372	Uridine-5'-monophosphate	0.01	0.01	0.04	0.02	0.06	0.03		
X00379	alpha-Lactose monohydrate	0.67	0.44	0.55	0.47	0.65	0.53		
X00389	gamma-Amino-n-butyric acid	5.37	2.60	3.63	3.13	2.55	1.80		
X00392	6-Aminohexanoic acid	0.70	0.73	1.21	1.21	0.88	1.15		
X00416	Keracyanin Chloride	1.69	3.21	3.72	2.26	2.02	1.39		
X00419	Isorhamnetin-3-O-glucoside	1.75	4.03	9.41	7.27	3.93	5.23		
X00422	Kaempferol-3-O-glucoside	10.58	20.55	23.24	21.48	12.59	20.79		
X00432	Hyperoside	0.72	2.51	6.10	4.89	2.59	3.60		
X00477	O-Acetyl-L-serine hydrochloride	0.50	0.91	0.51	0.41	0.50	0.59		
X00502	L-Saccharopine	0.19	0.31	0.44	0.32	0.21	0.26		
X00675	5'-Deoxy-5'-Methylthioadenosine	1.94	1.71	1.29	1.61	2.49	1.43		
X00695	L-allo-threonine	2.18	2.48	2.67	2.28	3.23	2.36		
X00755	5-Aminovaleric acid	2.96	2.50	3.47	2.95	3.86	2.96		

X00797	L-Threonic acid hemicalciums alt	1.01	0.71	0.91	0.65	0.80	0.75		
X00849	Hesperidin	0.06	0.28	0.38	0.16	0.26	0.32		
X00853	Luteolin-3',7-di-O-glucoside	4.79	10.31	12.10	10.62	7.04	10.64		
X00854	Luteolin-4'-O-glucoside	23.39	46.78	56.18	48.22	29.13	47.02		
X00860	Neohesperidin	0.13	0.54	0.74	0.33	0.56	0.64		
X00865	Poncirin	0.04	0.13	0.14	0.08	0.10	0.08		
X00906	Cysteinylglycine	0.77	0.68	0.87	0.54	1.77	1.11		
X00907	DL-Homocysteine	0.02	0.02	0.01	0.01	0.02	0.02		
X00921	Kaempferol-3-Rhamnoside-4"-Rhamnoside,-7-Rhamnoside	0.27	0.15	0.16	0.11	0.20	0.28		
X00924	Kaempferol-3-Glucuronide	33.51	31.71	35.49	26.00	26.48	29.25		
X00933	Quercetin-3-Glucuronide	12.99	14.85	18.83	12.99	13.53	16.46		
X00943	alpha-Methyl-DL-histidine dihydrochloride	0.05	0.03	0.03	0.01	0.06	0.01		
X00971	DL-5-Hydroxylysine hydrochloride	0.02	0.01	0.01	0.02	0.01	0.02		
X00986	L-Anserine	0.03	0.05	0.06	0.07	0.04	0.07		
X01016	Choline chloride	45.14	37.44	34.69	35.60	31.12	33.71		
X01026	Trigonelline hydrochloride	1.87	1.55	2.42	2.84	2.54	2.43		
X01097	DL-Pipecolic acid	2.63	6.58	5.52	3.28	6.40	2.58		
X01098	Maleic acid	0.12	0.07	0.06	0.07	0.03	0.06		
X01099	D-(+)-Raffinose pentahydrate	0.94	0.45	0.40	0.79	0.48	1.00		
X01144	S-Methyl-L-cysteine	0.70	0.72	0.87	0.72	0.50	0.65		
X01218	Petunidin-3-O-beta-glucopyranoside	3.69	2.71	3.33	5.89	2.53	5.10		
X01219	Quercetin-3,4'-O-di-beta-glucopyranoside	0.10	0.62	0.97	0.70	0.51	0.53		
X01220	Cyanidin-3-O-(2"-O-beta-xylopyranosyl-beta-glucopyranoside)	0.67	2.64	2.28	1.79	0.77	1.33		
X01223	Delphinidin-3-O-(6"-O-alpha-rhamnopyranosyl-beta-glucopyranoside)	0.97	1.98	3.25	1.81	1.65	2.03		
X01224	Delphinidin-3-O-(2"-O-beta-xylopyranosyl-beta-glucopyranoside)	0.18	0.21	0.46	0.47	0.22	0.38		
X01225	Cyanidin-3-O-(2"-O-beta-xylopyranosyl-beta-glucopyranoside)-5-O-beta-glucopyranoside	0.48	0.24	0.27	0.39	0.24	0.29		
X10002 4	L-Leucine, (Cell Culture Reagent, Crystalline)	0.73	1.02	1.56	1.69	1.09	1.77		
X10002 5	L-Isoleucine	0.61	0.70	1.26	1.12	0.80	1.21		
X10002 7	Methionine sulfoxide	0.20	0.33	0.49	0.42	0.30	0.33		
X10003 9	Luteolin 7-O-glucuronide	34.69	32.77	40.96	27.37	27.06	24.01		
X10004 3	2i_Leu_Ile	6.50	8.85	14.26	14.29	9.62	14.64		
X10004 4	2i_Gln_Lys	19.97	70.24	51.02	34.62	84.75	29.19		

X200004	3i_Isorhamnetin-3-O-rutinoside_Isorhamnetin-3-Glucoside-6"-Rhamnoside_Isorhamnetin-3-Galactoside-6"-Rhamnoside	2.62	5.17	7.20	4.67	3.46	4.57		
X200007	2i_Cyanidin-3,5-di-O-glucoside chloride_Cyanidin-3-O-(2"-O-beta-glucopyranosyl-beta-glucopyranoside)	5.52	10.58	12.36	12.30	7.72	11.56		
X200011	2i_Ideain chloride_Cyanidin-3-glucoside chloride	20.52	47.29	53.51	47.14	27.64	46.43		
X200012	2i_Maritimein_luteolin-7-O-glucoside	18.31	36.22	42.25	38.84	22.73	36.34		
X200017	2i_Syringetin-3-O-glucoside_Syringetin-3-O-galactoside	0.01	0.97	1.94	1.36	0.94	1.05		
X200029	2i_alpha-D-Glucose-1-phosphate dipotassium salt dihydrate_alpha-D-Galactose-1-phosphate dipotassium salt pentahydrate	0.12	0.14	0.16	0.11	0.16	0.06		
X200030	2i_D-Mannose-6-phosphate bariums salt hydrate_D-Mannose 6-phosphate mono sodiums salt	0.07	0.02	0.12	0.04	0.17	0.07		
X200031	4i_D-Fructose-6-phosphate disodiums salt hydrate_D-Glucose-6-phosphate sodiums salt_alpha-D-(+)-mannose-1-phosphate sodiums salt hydrate_alpha-D-(+)Mannose 1-phosphate bis(cyclohexylammonium) salt	0.03	0.07	0.12	0.05	0.17	0.07		
X200034	2i_D-(+)-Galactosamine hydrochloride_D-(+)-Glucosamine hydrochloride	0.02	0.09	0.09	0.04	0.09	0.08		
X200042	2i_D-(+)-Cellobiose_Lactulose	0.72	0.52	0.62	0.57	0.73	0.60		
X200043	6i_Melibiose hydrate_D-(+)-Turanose_Isomaltose_Gentiobiose_MelibiosePalatinose Monohydrate	4.40	3.27	3.93	3.71	4.79	3.87		
X200047	4i_L(+)-Arginine HCl_N-alpha-Acetyl-L-ornithine_L-Citrulline	1.36	4.38	6.28	4.83	8.02	6.66		
X200054	DL-Cysteine	0.02	0.01	0.01	0.01	0.03	0.01		
X200055	2i_Nicotinamide_Niacinamide	0.51	0.70	0.63	0.66	0.59	0.50		
X200057	2i_L-Alanine_Sarcosine	4.52	8.78	12.71	6.85	8.32	7.08		
X200060	2i_L-Norvaline_L-Valine	4.63	4.17	5.37	4.44	6.63	4.73		
X200061	3i_L-Threonine_alpha-Methyl-DL-serine_L-Homoserine	2.19	2.43	2.65	2.31	3.67	2.38		
X200063	3i_L-2-Aminobutyric acid_N,N-Dimethylglycine hydrochloride_N-Methyl-DL-Alanine	8.81	7.43	6.88	7.42	6.69	6.88		
X200068	DL-Malic acid	3.82	2.16	2.17	1.75	1.71	1.91		

X20007 2	L-CarnitineHCl	0.01	0.03	0.06	0.01	0.02	0.04		
X20007 3	DL-2-Aminoadipic Acid	0.13	0.09	0.12	0.11	0.28	0.15		
X20008 2	L-Lysine HCl	20.02	70.29	51.19	33.82	84.42	29.60		
X20008 5	2i_L-Norleucine_D-Alloisoleucine	6.43	8.69	12.84	14.02	8.97	14.91		
X20008 7	2i_Rutin_Quercetin-3-O-b-glucopyranosyl-7-O-a-rhamnopyranoside	0.46	1.45	2.07	1.10	1.57	1.82		
X20008 9	2i_D-(+)-Melezitose monohydrate_1-Kestose	0.81	0.51	0.37	0.80	0.43	0.92		
X26000 2	gamma-Glu-PRENC SO	1.05	0.83	0.68	0.77	1.18	1.04		
X26000 6	MCSO	6.62	0.41	0.40	1.19	4.97	1.27		
X26000 7	Alliin	27.88	13.53	21.06	14.96	48.93	21.65		



**Supplementary Table S3.** Gradient condition for mass spectrometry analysis

Time (min)	Flow ( $\mu\text{L} \cdot \text{min}^{-1}$ )	A (%)	B (%)
0.25	0.24	99.9	0.1
0.4	0.24	91	9
0.8	0.24	83	17
1.9	0.24	0.1	99.9
2.1	0.24	0.1	99.9
2.11	0.24	99.9	0.1
2.7	stope		

LC column: ACQUITY UPLC HSS T3 Column, 100 Å, 1.8  $\mu\text{m}$ , 1 mm  $\times$  50 mm (Waters)

Column oven temperature at 30°C

Mobile phase A: 0.1% v/v formic acid in water

Mobile phase B: 0.1% v/v formic acid in acetonitrile