Supplemental Data for:

Richter, C.L., A.D. Kennedy, L. Guo, and N. Dokoozlian
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	Concentration								Identifier		
Compound	Day 4	Day 9	Day 15	Super pathway	Subpathway	Platform	RI	Mass	CAS	PUBCHEM	KEGG
2-Aminobutyrate	5.33	0.89	0.26	Amino acid	Butanoate metabolism	GC-MS	1215.7	130	1492-24-6;	4,396,916,971,251	C02261
2-Hydroxy-3-methylvalerate	1.04	0.97	0.50	Amino acid	Valine, leucine and isoleucine metabolism	GC-MS	1281	159.09	488-15-3;	164623	
3-(4-Hydroxyphenyl)lactate (HPLA)	0.78	0.70	1.32	Amino acid	Phenylalanine & tyrosine metabolism	LC-MS Neg	1395	181.1	6482-98-0;	9378	C03672
3-Hydroxyanthranilate	1.07	0.97	0.97	Amino acid	Tryptophan metabolism	LC-MS Pos	2280	154.1	548-93-6;	86	C00632
3-Methylhistidine	1.15	0.63	0.63	Amino acid	Histidine metabolism	GC-MS	1799.7	218.1	368-16-1;	649,696,971,061	C01152
4-Acetamidobutanoate	1.03	0.39	0.45	Amino acid	Guanidino and acetamido metabolism	LC-MS Pos	1724	146.1	3025-96-5;	18189	C02946
4-Guanidinobutanoate	0.88	0.95	0.56	Amino acid	Guanidino and acetamido metabolism	LC-MS Pos	1085	146.1	463-003;463-00-3;	500	C01035
5-Aminovalerate	7.53	0.92	0.08	Amino acid	Urea cycle; arginine and proline metabolism	GC-MS	1620.8	174	660-88-8;	6,992,101,138	C00431
5-Methylthioadenosine (MTA)	1.65	0.78	0.10	Amino acid	Polyamine metabolism	LC-MS Pos	2427	298.1	2457-80-9;	439176	C00170
5-Oxoproline	0.67	1.63	2.12	Amino acid	Glutathione metabolism	LC-MS Neg	744	128.2	98-79-3;	7405	C01879
Alanine	2.34	1.10	0.09	Amino acid	Alanine and aspartate metabolism	GC-MS	1147.6	115.9	56-41-7;	59,507,311,724	C00041
allo-Threonine	5.16	0.79	0.09	Amino acid	Glycine, serine, and threonine metabolism	GC-MS	1417.8	219	28954-12-3;	992,896,995,276	C05519
a-Hydroxyisocaproate	0.82	0.95	0.25	Amino acid	Valine, leucine, and isoleucine metabolism	LC-MS Neg	1854	131.2	10303-64-7;	83697	C03264
a-Hydroxyisovalerate	0.95	0.37	0.17	Amino acid	Valine, leucine, and isoleucine metabolism	GC-MS	1208	145.1	600-37-3;	99823	
Anthranilate	3.67	0.37	0.44	Amino acid	Tryptophan metabolism	LC-MS Pos	3213	138.1	118-92-3;	3,734,162,227	C00108
Arginine	2.42	1.29	0.43	Amino acid	Urea cycle; arginine and proline metabolism	LC-MS Neg	728	173.2	1119-34-2;	5,246,487,232	C00062
Argininosuccinate	2.43	1.10	0.58	Amino acid	Urea cycle; arginine and proline metabolism	LC-MS Pos	689	291.2	156637-58-0;	828	C03406
Asparagine	1.02	1.30	0.11	Amino acid	Alanine and aspartate metabolism	GC-MS	1617.5	188	70-47-3;	62,676,992,089	C00152
Aspartate	2.14	0.75	0.05	Amino acid	Alanine and aspartate metabolism	GC-MS	1529.7	232	56-84-8;	5960	C00049
b-Alanine	2.05	0.71	0.43	Amino acid	Alanine and aspartate metabolism	GC-MS	1451.8	174	56-41-7;107-95-9;	2,394,755,801	C00099
b-Hydroxypyruvate	0.64	0.96	1.61	Amino acid	Glycine, serine, and threonine metabolism	GC-MS	1425.1	221	3369-79-7;	964	C00168
Betaine	1.02	0.70	1.56	Amino acid	Glycine, serine, and threonine metabolism	LC-MS Pos	721	118.2	107-43-7;	247	
Citramalate	1.11	1.51	1.73	Amino acid	Valine, leucine, and isoleucine metabolism	GC-MS	1490.7	247	6236-10-8;	1081	C02612,C00815

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Compound	Day 4	Day 9	Day 15	Super pathway	Subpathway	Platform	RI	Mass	CAS	PUBCHEM	KEGG
Cystathionine	1.78	0.93	0.11	Amino acid	Cysteine, methionine, SAM, taurine metabolism	GC-MS	1979.6	218.1	535-34-2;	4,083,111,834	C02291
Cysteine	1.07	1.04	0.50	Amino acid	Cysteine, methionine, SAM, taurine metabolism	GC-MS	1560.1	218	52-90-4;56-89-3;	58,626,419,722	C00097
Dimethylarginine (ADMA + SDMA)	0.80	1.10	0.20	Amino acid	Urea cycle; arginine and proline metabolism	LC-MS Pos	812	203.2		123831	C03626
g-Aminobutyrate (GABA)	0.78	3.12	0.61	Amino acid	Glutamate metabolism	GC-MS	1539.7	304.1	56-12-2;	6,992,099,119	C00334
Gentisate	0.50	1.04	1.41	Amino acid	Phenylalanine and tyrosine metabolism	LC-MS Neg	1460	153.1	490-79-9;	3469	C00628
Glutamate	4.28	0.95	0.82	Amino acid	Glutamate metabolism	LC-MS Pos	700	148.1	56-86-0;	611	C00025
Glutamate, g-methyl ester	8.91	1.23	0.11	Amino acid	Glutamate metabolism	LC-MS Pos	1062	162.1	1499-55-4;	73913	
Glutamine	0.87	1.11	0.43	Amino acid	Glutamate metabolism	LC-MS Pos	684	147.2	56-85-9;	69,920,865,961	C00064
Glutarate (pentanedioate)	1.06	1.93	0.28	Amino acid	Lysine metabolism	GC-MS	1433.6	261	110-94-1;	4418048	C00489
Glutathione, oxidized (GSSG)	1.88	0.98	0.16	Amino acid	Glutathione metabolism	LC-MS Pos	1535	613.1	103239-24-3;	6,535,911,215,652	C00127
Glutathione, reduced (GSH)	1.33	0.82	0.09	Amino acid	Glutathione metabolism	LC-MS Pos	1274	308.1	70-18-8;	124886	C00051
Glycine	4.21	0.82	0.07	Amino acid	Glycine, serine, and threonine metabolism	GC-MS	1166	101.9	56-40-6;	5,257,127,750	C00037
Histidine	2.66	0.72	0.04	Amino acid	Histidine metabolism	GC-MS	1837.3	154	5934-29-2;	7,733,651,426	C00135
Homocysteine	2.32	0.86	0.08	Amino acid	Cysteine, methionine, SAM, taurine metabolism	GC-MS	1648.2	234	454-29-5;	778	C00155
Homoserine (homoserine lactone)	2.18	1.00	0.54	Amino acid	Glycine, serine, and threonine metabolism	GC-MS	1471	218.1	672-15-1;	126,476,971,022	C00263,C02926
Homoserine lactone	1.07	1.15	0.12	Amino acid	Glycine, serine, and threonine metabolism	GC-MS	1296	130	2185-02-6;	445963	C02926
Imidazole lactate	1.88	0.64	0.74	Amino acid	Histidine metabolism	LC-MS Pos	778	157.1	14403-45-3;	440129	C05568
Isoleucine	3.20	1.06	0.22	Amino acid	Valine, leucine, and isoleucine metabolism	LC-MS Pos	1614	132.1	73-32-5;	791	C00407
Kynurenate	7.86	0.58	1.10	Amino acid	Tryptophan metabolism	LC-MS Neg	2243	188.1	492-27-3;	3845	C01717
Kynurenine	20.05	1.28	0.33	Amino acid	Tryptophan metabolism	LC-MS Pos	1902	209.1	2922-83-0;	1,611,666,971,029	C00328
Leucine	1.85	1.07	0.38	Amino acid	Valine, leucine, and isoleucine metabolism	LC-MS Pos	1674	132.2	61-90-5;	70,457,986,106	C00123
Lysine	2.70	0.63	0.03	Amino acid	Lysine metabolism	GC-MS	1679	156.1	56-87-1;	5962	C00047
Methionine	2.97	1.07	0.37	Amino acid	Cysteine, methionine, SAM, taurine metabolism	LC-MS Pos	1252	150.1	63-68-3;	69,920,876,137	C00073
N-Acetylalanine	0.74	1.11	0.18	Amino acid	Alanine and aspartate metabolism	LC-MS Neg	882	130.1	97-69-8;	88064	C02847

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Compound	Day 4	Day 9	Day 15	Super pathway	Subpathway	Platform	RI	Mass	CAS	PUBCHEM	KEGG
N-Acetylarginine	4.90	1.59	0.12	Amino acid	Urea cycle; arginine and proline metabolism	LC-MS Neg	1149	215.2	155-84-0;	674,271,615,663	C02562
N-Acetylasparagine	0.99	1.50	0.58	Amino acid	Alanine and aspartate metabolism	LC-MS Pos	974	175.1	4033-40-3;	99715	
N-Acetylglutamine	2.44	1.18	0.30	Amino acid	Glutamate metabolism	LC-MS Pos	1204	189.1	2490-97-3;	182230	C02716
N-Acetylglycine	1.78	1.04	0.47	Amino acid	Glycine, serine, and threonine metabolism	GC-MS	1396.4	143.9	543-24-8;	10972	
N-Acetylhistidine	2.28	1.36	0.31	Amino acid	Histidine metabolism	LC-MS Pos	843	198.1	39145-52-3;	75619	C02997
N-Acetylleucine	4.75	0.83	1.07	Amino acid	Valine, leucine, and isoleucine metabolism	LC-MS Pos	3444	174.1	1188-21-2;	70912	C02710
N-Acetylmethionine	2.77	0.95	0.45	Amino acid	Cysteine, methionine, SAM, taurine metabolism	LC-MS Neg	1805	190.1	65-82-7;	448580	C02712
N-Acetylphenylalanine	1.42	0.23	0.39	Amino acid	Phenylalanine and tyrosine metabolism	LC-MS Pos	3563	208.1	2018-61-3;	74839	C03519
N-Acetylproline	2.50	0.85	0.52	Amino acid	Urea cycle; arginine-, proline-, metabolism	LC-MS Pos	2184	158.1	1074-79-9;	322640	
N-Acetyltyrosine	2.92	0.38	0.37	Amino acid	Phenylalanine and tyrosine metabolism	LC-MS Neg	1677	222.2	537-55-3;	68310	
N_6-Acetyllysine	0.88	0.54	0.10	Amino acid	Lysine metabolism	LC-MS Pos	1134	189.1	692-04-6;	699,197,892,832	C02727
Norophthalmate	0.99	2.04	0.43	Amino acid	Glutathione metabolism	LC-MS Pos	989	276.1	1116-21-8;	5489007	
Ophthalmate	2.31	0.57	0.16	Amino acid	Glutathione metabolism	LC-MS Pos	1457	290.1	495-27-2;	9817431	
Ornithine	4.12	1.52	0.15	Amino acid	Urea cycle; arginine and proline metabolism	GC-MS	1763.8	141.9	3184-13-2;	6262	C00077
p-Toluic Acid	0.93	0.57	0.71	Amino acid	Phenylalanine and tyrosine metabolism	GC-MS	1400	193	99-94-5;	7470	C01454
Phenylalanine	2.53	0.93	0.38	Amino acid	Phenylalanine and tyrosine metabolism	LC-MS Pos	2056	166.1	63-91-2;	69,256,656,140	C00079
Phenyllactate (PLA)	0.87	1.07	0.74	Amino acid	Phenylalanine and tyrosine metabolism	LC-MS Neg	2237	165.1	828-01-3;	3848	C05607
Pipecolate	1.70	0.76	0.23	Amino acid	Lysine metabolism	GC-MS	1396.1	156	4043-87-2;	849	C00408
Proline	1.69	1.00	0.96	Amino acid	Urea cycle; arginine and proline metabolism	LC-MS Pos	796	116.1	147-85-3;	1,457,426,971,047	C00148
Pyroglutamine	0.86	0.82	1.03	Amino acid	Glutamate metabolism	LC-MS Pos	764	129.2		134508	
S-Adenosylhomocysteine (SAH)	6.24	0.83	0.35	Amino acid	Cysteine, methionine, SAM, taurine metabolism	LC-MS Pos	1480	193.2	979-92-0;		C00021
S-Adenosylmethionine (SAM)	0.62	1.45	0.63	Amino acid	Cysteine, methionine, SAM, taurine metabolism	LC-MS Pos	676	399.1	24346-00-7;		
S-Methylglutathione	7.22	1.21	0.29	Amino acid	Glutathione metabolism	LC-MS Pos	1610	322.1	2922-56-7;	3605667	C11347

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	Concentration								Identifier		
Compound	Day 4	Day 9	Day 15	Super pathway	Subpathway	Platform	RI	Mass	CAS	PUBCHEM	KEGG
Saccharopine	0.60	1.06	0.75	Amino acid	Lysine metabolism	LC-MS Pos	695	277.1	997-68-2;	160556	C00449
Serine	3.73	1.06	0.05	Amino acid	Glycine, serine, and threonine metabolism	GC-MS	1389.1	204	56-45-1;	59,516,857,581	C00065
Spermidine	1.25	1.14	0.47	Amino acid	Polyamine metabolism	LC-MS Pos	533	146.2	124-20-9;	1102	C00315
Threonine	3.83	0.91	0.43	Amino acid	Glycine, serine, and threonine metabolism	LC-MS Pos	713	120.1	72-19-5;	69,710,196,288	C00188
Hydroxyproline	2.20	0.98	0.66	Amino acid	Urea cycle; arginine and proline metabolism	GC-MS	1537	140	51-35-4;	58,106,971,053	C01157
Tryptophan	2.27	0.85	0.42	Amino acid	Tryptophan metabolism	LC-MS Pos	2445	205.1	73-22-3;	69,235,166,305	C00078
Tyrosine	4.35	0.89	0.31	Amino acid	Phenylalanine and tyrosine metabolism	LC-MS Pos	1516	182.1	60-18-4;	60,576,942,100	C00082
Urea	103.72	0.66	0.90	Amino acid	Urea cycle; arginine and proline metabolism	GC-MS	1223.9	171	57-13-6;	117,616,150,869	C00086
Valine	3.19	0.98	0.15	Amino acid	Valine, leucine, and isoleucine metabolism	LC-MS Pos	1040	118.1	72-18-4;	69,710,186,287	C00183
Xanthurenate	0.60	1.08	1.62	Amino acid	Tryptophan metabolism	LC-MS Pos	2690	206.1	59-007;	5699	C02470
2,3-Butanediol	0.90	0.54	0.28	Carbohydrate	Glycolysis, gluconeogenesis, pyruvate metabolism	GC-MS	1075	116.9	24347-58-8;		C03044
2-Isopropylmalate	0.20	1.11	1.02	Carbohydrate	Glycolysis, gluconeogenesis, pyruvate metabolism	LC-MS Pos	2917	194.1	3237-44-3;	77	C02504
3-Phosphoglycerate	1.60	1.51	0.09	Carbohydrate	Glycolysis, gluconeogenesis, pyruvate metabolism	GC-MS	1756	299	80731-10-8;		C00597
Arabinose	0.26	0.99	1.17	Carbohydrate	Nucleotide sugars, pentose metabolism	GC-MS	1631.6	217	28697-53-2;	66308	C00181
Arabitol	1.24	0.53	0.23	Carbohydrate	Nucleotide sugars, pentose metabolism	GC-MS	1687.5	217	488-82-4;	94154	C00474
Dihydroxyacetone phosphate (DHAP)	0.22	0.64	0.22	Carbohydrate	Glycolysis, gluconeogenesis, pyruvate metabolism	GC-MS	1737	315.1	102783-56-2;	4643300	C00111
Erythronate	1.25	0.90	0.91	Carbohydrate	Amino-sugar metabolism;	GC-MS	1546.9	292.1	13752-84-6;	2781043	
Fructose	0.25	30.06	1.52	Carbohydrate	fructose, mannose, galactose, starch, and sucrose metabolism	GC-MS	1758	217	57-48-7;	5984	C00095
Fructose 6-phosphate	0.67	24.05	0.47	Carbohydrate	Glycolysis, gluconeogenesis, pyruvate metabolism	GC-MS	1994.9	315.1	103213-47-4;		C05345
Galactinol	1.08	1.01	1.02	Carbohydrate	Fructose, mannose, galactose, starch, and sucrose metabolism	GC-MS	2226.1	433.3	16908-86-4;		C01235
Galactitol (dulcitol)	0.55	1.11	0.54	Carbohydrate	Fructose, mannose, galactose, starch, and sucrose metabolism	GC-MS	1849.2	319.1	608-66-2;	11850	C01697

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Galactose	0.63	1.00	1.67	Carbohydrate	Fructose, mannose, galactose, starch, and sucrose metabolism	GC-MS	1793.8	203.9	59-23-4;	3037556	C01582
Glucose	0.07	6.70	0.59	Carbohydrate	Glycolysis, gluconeogenesis, pyruvate metabolism	GC-MS	1866.8	217.1	50-99-7;	79025	C00293
Glucose 1-phosphate	0.03	1.23	0.03	Carbohydrate	Glycolysis, gluconeogenesis, pyruvate metabolism	GC-MS	2017	299.1	56401-20-8;	65533	C00103
Glucose 6-phosphate	0.07	2.40	0.00	Carbohydrate	Glycolysis, gluconeogenesis, pyruvate metabolism	GC-MS	2042.7	387.2	103192-55-8;		C00668
Glycerate	0.79	1.95	0.98	Carbohydrate	Glycolysis, gluconeogenesis, pyruvate metabolism	GC-MS	1360.7	189	600-19-1;	752	C00258
Isobar: fructose 1,6-diphosphate, glucose 1,6-diphosphate, myo-inositol 1,4 or 1,3-diphosphate	0.29	13.81	0.19	Carbohydrate	Glycolysis, gluconeogenesis, pyruvate metabolism	LC-MS Neg	572	339			
Isobar: ribulose 5-phosphate, Xylulose 5-phosphate	0.08	1.31	0.04	Carbohydrate	Nucleotide sugars, pentose metabolism	GC-MS	1935	357.2			
Isomaltose	0.74	1.08	0.75	Carbohydrate	Fructose, mannose, galactose, starch, and sucrose metabolism	GC-MS	2221.8	204.1	499-40-1;	439193	C00252
Lactate	0.34	1.19	0.71	Carbohydrate	Glycolysis, gluconeogenesis, pyruvate metabolism	GC-MS	1102.8	116.9	79-33-4;	612	C00186
Mannitol	0.99	4.47	0.36	Carbohydrate	Fructose, mannose, galactose, starch, and sucrose metabolism	GC-MS	1839	319.1	69-65-8;	6251	C00392
Mannose	0.80	1.87	0.92	Carbohydrate	Fructose, mannose, galactose, starch, and sucrose metabolism	GC-MS	1753.5	203.9	3458-28-4;	161658	C00159
Mannose 6-phosphate	0.64	2.98	0.06	Carbohydrate	Fructose, mannose, galactose, starch, and sucrose metabolism	GC-MS	2035.9	387.2	70442-25-0;104872-94-8;		C00275
N-Acetylglucosamine	0.85	0.84	1.09	Carbohydrate	Amino-sugar metabolism	GC-MS	1903.3	245	7512-17-6;	24139	C00140
Pyruvate	1.21	0.64	0.69	Carbohydrate	Glycolysis, gluconeogenesis, pyruvate metabolism	GC-MS	1130.6	217	127-17-3;	107735	C00022
Rhamnose	0.75	0.96	1.14	Carbohydrate	Fructose, mannose, galactose, starch, and sucrose metabolism	GC-MS	1669.4	204	10030-85-0;	19233	C00507
Ribitol	1.02	0.66	0.10	Carbohydrate	Nucleotide sugars, pentose metabolism	GC-MS	1692.4	217	488-81-3;		C00474
Ribose	0.08	1.09	0.99	Carbohydrate	Nucleotide sugars, pentose metabolism	GC-MS	1639.2	204	50-69-1;	5311110	C00121
Ribulose	0.39	1.71	0.52	Carbohydrate	Nucleotide sugars, pentose metabolism	GC-MS	1662	306.1	488-84-6;	79021	C00309
Sedoheptulose-7-phosphate	0.32	2.69	0.26	Carbohydrate	Nucleotide sugars, pentose metabolism	GC-MS	2070	691.35	2646-35-7;	616	C05382

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Compound	Day 4	Day 9	Day 15	Super pathway	Subpathway	Platform	RI	Mass	CAS	PUBCHEM	KEGG
Sorbitol	0.77	1.05	0.46	Carbohydrate	Fructose, mannose, galactose, starch, and sucrose metabolism	GC-MS	1843	319.1	6706-59-8;	107428	C00794
Threitol	1.07	0.90	0.73	Carbohydrate	Nucleotide sugars, pentose metabolism	GC-MS	1513	217.1	2418-52-2;	169019	C16884
Trehalose	0.96	1.37	0.09	Carbohydrate	Fructose, mannose, galactose, starch, and sucrose metabolism	GC-MS	2174.9	361.2	6138-23-4;	7427	C01083
UDP-glucose	0.70	0.53	0.53	Carbohydrate	Nucleotide sugars, pentose metabolism	GC-MS	1986	243.1	117756-22-6;	8629	C00029
Xylitol	0.67	0.71	0.37	Carbohydrate	Nucleotide sugars, pentose metabolism	GC-MS	1677.6	307.2	87-99-0;	6912	C00379
Xylonate	1.12	0.88	0.57	Carbohydrate	Nucleotide sugars, pentose metabolism	GC-MS	1722	292	73686-31-7;	6602431	C00502,C05411
Xylulose	0.60	1.44	0.43	Carbohydrate	Nucleotide sugars, pentose metabolism	GC-MS	1668	306.1	551-84-8;	5289590	C00310
2,3-Dihydroxyisovalerate	0.64	0.86	0.88	Cofactors and vitamins	Pantothenate and CoA metabolism	GC-MS	1422	131	1756-18-9;	677	C04039
3′-Dephosphocoenzyme A	0.37	1.28	0.12	Cofactors and vitamins	Pantothenate and CoA metabolism	LC-MS Neg	2010	686.2	3633-59-8;	444485	C00882
5-Aminolevulinate	0.68	1.08	0.74	Cofactors and vitamins	Hemoglobin and porphyrin metabolism	LC-MS Pos	711	132	5451-09-2;	1,377,048,523	C00430
Acetyl CoA	0.50	1.11	0.48	Cofactors and vitamins	Pantothenate and CoA metabolism	LC-MS Neg	1900	808.1	102029-73-2;	444493	C00024
Adenosine 5′-diphosphoribose (ADP-Ribose)	0.41	1.74	1.50	Cofactors and vitamins	Nicotinate and nicotinamide metabolism	LC-MS Neg	964	558.1	68414-18-6;	4475880	C00301
Ascorbate (vitamin C)	0.98	0.05	0.05	Cofactors and vitamins	Ascorbate and aldarate metabolism	GC-MS	1850.1	332.1	134-03-2;		C00072
CoA	0.66	1.74	0.58	Cofactors and vitamins	Pantothenate and CoA metabolism	LC-MS Neg	1600	766.1	85-61-0;18439-24-2;	317	C00010
Coproporphyrin III	0.70	1.09	4.39	Cofactors and vitamins	Hemoglobin and porphyrin metabolism	LC-MS Pos	5143.1	655.4	14643-66-4;		C05770
FAD	3.35	1.00	0.57	Cofactors and vitamins	Riboflavin metabolism	LC-MS Neg	2413	784.1	146-14-5;84366-81-4;	643975	C00016
FMN	4.24	0.87	0.57	Cofactors and vitamins	Riboflavin metabolism	LC-MS Neg	2395	455.1	130-40-5;	710	C00061
Nicotinamide	1.34	0.60	1.31	Cofactors and vitamins	Nicotinate and nicotinamide metabolism	LC-MS Pos	1267	123.1	98-92-0;	936	C00153
NAD^+	1.79	0.57	0.20	Cofactors and vitamins	Nicotinate and nicotinamide metabolism	LC-MS Pos	1370	664	53-84-9;	5893	C00003
NADH	4.42	0.17	0.17	Cofactors and vitamins	Nicotinate and nicotinamide metabolism	LC-MS Neg	1554	664.1	58-68-4;606-68-8;	439153	C00004
Nicotinamide ribonucleotide (NMN)	1.67	0.95	0.29	Cofactors and vitamins	Nicotinate and nicotinamide metabolism	LC-MS Pos	886	335.1	1094-61-7;	14180	C00455

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	Concentration								Identifier		
Compound	Day 4	Day 9	Day 15	Super pathway	Subpathway	Platform	RI	Mass	CAS	PUBCHEM	KEGG
Nicotinamide riboside	0.18	2.78	0.03	Cofactors and vitamins	Nicotinate and nicotinamide metabolism	LC-MS Pos	955	255.1	1341-23-7;		
Nicotinate ribonucleoside	0.56	0.51	0.93	Cofactors and vitamins	Nicotinate and nicotinamide metabolism	LC-MS Pos	1105	256	2625-49-2;	161233	
Pantothenate (vitamin B5)	1.01	0.52	0.40	Cofactors and vitamins	Pantothenate and coa metabolism	LC-MS Pos	2218	220.1	137-08-6;	6613	C00864
Phosphopantetheine	11.08	0.57	0.41	Cofactors and vitamins	Pantothenate and coa metabolism	LC-MS Neg	1624	357.2	NA;	115254	C01134
Pyridoxal	1.77	0.72	0.91	Cofactors and vitamins	Pyridoxal metabolism	LC-MS Pos	1210	168.1	65-22-5;	1050	C00250
Pyridoxine (vitamin B6)	10.10	0.82	1.27	Cofactors and vitamins	Vitamin B6 metabolism	LC-MS Pos	1386	170.1	58-56-0;	1054	C00314
Riboflavin (vitamin B2)	1.03	1.06	0.82	Cofactors and vitamins	Riboflavin metabolism	LC-MS Pos	3111	377.2	83-88-5;	493570	C00255
Thiamin (vitamin B1)	1.05	1.49	0.44	Cofactors and vitamins	Thiamine metabolism	LC-MS Neg	1699	263.1	59-43-8;		
Threonate	1.06	0.79	1.01	Cofactors and vitamins	Ascorbate and aldarate metabolism	GC-MS	1560.7	292.1	70753-61-6;	151152	C01620
Acetylphosphate	1.55	0.96	0.15	Energy	Oxidative phosphorylation	GC-MS	1263	211	94249-01-1;	186	C00227
a-Ketoglutarate	0.21	1.27	8.60	Energy	Krebs cycle	GC-MS	1779	419.1	305-72-6;328-50-7;22202-68-2;	51	C00026
cis-Aconitate	0.08	1.84	0.14	Energy	Krebs cycle	LC-MS Neg	603	173.1	585-84-2;	643757	C00417
Citrate	0.14	1.61	0.95	Energy	Krebs cycle	GC-MS	1763.4	273.1	77-92-9;	311	C00158
Fumarate	0.92	0.94	0.16	Energy	Krebs cycle	GC-MS	1382.1	245	100-17-8;		C00122
Homocitrate	4.67	0.99	0.17	Energy	Krebs cycle	LC-MS Neg	568.8	205.1	3562-74-1;	439459	C01251
Isocitrate	0.07	0.92	1.06	Energy	Krebs cycle	LC-MS Pos	953	210	20226-99-7;	1198	C00311
Malate	0.46	1.12	1.25	Energy	Krebs cycle	GC-MS	1502	233	6915-15-7;	525	C00149
Phosphate	1.89	1.04	0.17	Energy	Oxidative phosphorylation	GC-MS	1307.7	298.9	7664-38-2;	1061	C00009
Succinate	0.98	0.86	0.56	Energy	Krebs cycle	LC-MS Neg	618	117.1	110-15-6;	1110	C00042
1,2-Propanediol	0.84	0.60	0.28	Lipid	Ketone bodies	GC-MS	1041	117	57-55-6;		C00717,C02912,C00583,C01506,C02917
1-Oleoyl-GPC (18:1)	1.14	0.20	0.20	Lipid	Lysolipid	LC-MS Pos	5700	522.4	19420-56-5;	16081932	
1-Palmitoleoyl-GPC (16:1)	1.57	0.05	0.04	Lipid	Lysolipid	LC-MS Pos	5524	494.3			
1-Palmitoylglycerol (16:0)	2.64	1.06	0.44	Lipid	Monoacylglycerol	GC-MS	2119.5	371.3	542-44-9;	14900	
1-Palmitoyl-GPC (16:0)	16.22	0.49	0.15	Lipid	Lysolipid	LC-MS Pos	5671	496.4	17364-16-8;	86554	
1-Palmitoyl-GPE (16:0)	7.14	0.54	0.45	Lipid	Lysolipid	LC-MS Pos	5635	454.2		9547069	
1-Palmitoyl-GPI (16:0)	9.70	1.48	0.54	Lipid	Lysolipid	LC-MS Neg	5573	571.3			
1-Stearoylglycerol (18:0)	1.66	1.08	0.44	Lipid	Monoacylglycerol	GC-MS	2186.6	399.4	123-94-4;	24699	D01947
1-Stearoyl-GPC (18:0)	5.92	0.53	0.22	Lipid	Lysolipid	LC-MS Pos	5844	524.4	19420-57-6;	497299	
1-Stearoyl-GPI (18:0)	5.08	1.53	0.18	Lipid	Lysolipid	LC-MS Neg	5800	599.4			
13-HODE + 9-HODE	1.02	1.05	0.27	Lipid	Fatty acid, monohydroxy	LC-MS Neg	5247	295.2			

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	Concentration								Identifier		
Compound	Day 4	Day 9	Day 15	Super pathway	Subpathway	Platform	RI	Mass	CAS	PUBCHEM	KEGG
2-Hydroxyglutarate	0.40	1.08	1.05	Lipid	Fatty acid, dicarboxylate	GC-MS	1576	247	40951-21-1;	43	C02630
2-Hydroxyoctanoate	3.68	0.88	0.18	Lipid	Fatty acid, monohydroxy	GC-MS	1473.6	187	617-73-2;	94180	
2-Hydroxypalmitate	0.57	0.76	0.29	Lipid	Fatty acid, monohydroxy	LC-MS Neg	5508	271.3	764-67-0;	92836	
2-Hydroxystearate	1.54	0.84	0.33	Lipid	Fatty acid, monohydroxy	LC-MS Neg	5705	299.4	629-22-1;	69417	C03045
2-Oleoyl-GPC (18:1)	4.46	0.46	0.46	Lipid	Lysolipid	LC-MS Pos	5640	522.4			
2-Oleoyl-GPE (18:1)	0.82	0.63	0.63	Lipid	Lysolipid	LC-MS Pos	5625	480.2			
2-Palmitoleoyl-GPC (16:1)	1.53	0.05	0.05	Lipid	Lysolipid	LC-MS Pos	5482	494.3			
2-Palmitoleoyl-GPE (16:1)	1.29	0.75	0.64	Lipid	Lysolipid	LC-MS Neg	5611	450.3			
2-Palmitoyl-GPC (16:0)	1.32	0.20	0.20	Lipid	Lysolipid	LC-MS Pos	5604	496.3			
2-Palmitoyl-GPE (16:0)	2.07	0.63	0.29	Lipid	Lysolipid	LC-MS Neg	5790	452.3			
2-Stearoyl-GPC (18:0)	1.47	0.53	0.53	Lipid	Lysolipid	LC-MS Pos	5780	524.4		10208382	
2-Stearoylglycerophosphoinositol	2.22	0.65	0.15	Lipid	Lysolipid	LC-MS Neg	5751.6	599.4			
3-Hydroxy-3-methylglutarate	1.00	0.53	0.37	Lipid	Mevalonate metabolism	GC-MS	1598.2	247	503-49-1;	5459993	C03761
3-Hydroxydecanoate	0.94	0.90	0.49	Lipid	Fatty acid, monohydroxy	LC-MS Neg	4681	187.2	5561-87-5;	26612	
3-Ketosphinganine	0.72	0.84	2.52	Lipid	Sphingolipid	LC-MS Pos	5218	300.4	18944-28-0;	631	C02934
4-Hydroxybutyrate (GHB)	0.68	0.99	0.11	Lipid	Fatty acid, monohydroxy	GC-MS	1277	233.1	502-85-2;	10413	C00989
Acetylcarnitine (C2)	1.05	0.50	0.20	Lipid	Carnitine metabolism	LC-MS Pos	1203	204.2	5080-50-2;	7045767	C02571
Acetylcholine	0.40	4.25	1.77	Lipid	Neurotransmitter	LC-MS Pos	866	146.1	60-32-1;	187	C01996
Arachidonate (20:4n6)	1.71	0.92	0.83	Lipid	Long-chain fatty acid	LC-MS Neg	5525	303.4	506-32-1;	444899	C00219
Azelate (nonanedioate; C9)	1.06	1.29	0.32	Lipid	Fatty acid, dicarboxylate	LC-MS Neg	1322	187.2	123-99-9;	2266	C08261
b-Sitosterol	2.02	1.27	1.08	Lipid	Sterol-steroid	GC-MS	2380.8	357.4	83-46-5;	222284	C01753
Caprate (10:0)	1.80	2.13	0.24	Lipid	Medium-chain fatty acid	LC-MS Neg	5092	171.2	112-37-8;	2969	C01571
Caproate (6:0)	4.59	1.45	0.14	Lipid	Medium-chain fatty acid	LC-MS Neg	2766	115.2	142-62-1;	8892	C01585
Caprylate (8:0)	2.07	1.30	0.33	Lipid	Medium-chain fatty acid	LC-MS Neg	4367	143.2	124-07-2;	379	C06423
Carnitine	1.05	0.99	0.52	Lipid	Carnitine metabolism	LC-MS Pos	702	162.2	461-05-2;	10917	
Cholate	0.73	2.19	4.28	Lipid	Bile acid metabolism	LC-MS Neg	5148	407.4	81-25-4;		C00695
Vaccenate (18:1n7)	1.24	1.24	1.96	Lipid	Long-chain fatty acid	GC-MS	1987	339.3	693-72-1;	5282761	C08367
Deoxycarnitine	1.07	0.61	0.40	Lipid	Carnitine metabolism	LC-MS Pos	759	146.1	6249-56-5;	725	C01181
Deoxycholate	0.79	1.62	1.36	Lipid	Bile acid metabolism	LC-MS Neg	5268	391.4	83-44-3;	440355	C04483
Ergosterol	3.91	0.61	1.23	Lipid	Sterol-steroid	GC-MS	2346.1	363.3	57-87-4;	444679	C01694
Ethanolamine	1.49	1.01	0.50	Lipid	Glycerolipid metabolism	GC-MS	1074	102	141-43-5;		C00189
Ethylpalmitate	0.27	1.86	2.29	Lipid	Fatty acid, ester	GC-MS	1882	101.04	628-97-7;	12366	
Ethyl stearate	0.05	1.05	2.35	Lipid	Fatty acid, ester	GC-MS	1977	101.04	111-61-5;	8122	
Glycerol	2.02	0.63	0.43	Lipid	Glycerolipid metabolism	GC-MS	1311	205	56-81-5;	753	C00116

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	Concentration								Identifier		
Compound	Day 4	Day 9	Day 15	Super pathway	Subpathway	Platform	RI	Mass	CAS	PUBCHEM	KEGG
Glycerol 3-phosphate (G3P)	1.34	0.73	0.09	Lipid	Glycerolipid metabolism	GC-MS	1719.7	357.1	29849-82-9;	754	C00093
Glycerophosphoethanolamine	1.81	1.33	0.08	Lipid	Glycerolipid metabolism	GC-MS	1906	357.1	33049-08-0;	123874	C01233
Glycerophosphorylcholine (GPC)	1.00	0.90	0.30	Lipid	Glycerolipid metabolism	LC-MS Pos	694	258.1	28319-77-9;	657272	C00670
Glycocholate	0.52	1.43	3.02	Lipid	Bile acid metabolism	LC-MS Neg	5104	464.4	475-31-0;863-57-0;	10140	C01921
Inositol 1-phosphate (I1P)	1.16	2.89	0.20	Lipid	Inositol metabolism	GC-MS	2057.8	318.1	106032-59-1;		
Lanosterol	2.74	1.48	2.41	Lipid	Sterol-steroid	GC-MS	2388	393.3	79-63-0;	246983	C01724
Laurate (12:0)	1.72	1.89	0.11	Lipid	Medium-chain fatty acid	LC-MS Neg	5288	199.3	143-07-7;	3893	C02679
Linoleate (18:2n6)	1.02	2.25	0.55	Lipid	Essential fatty acid	LC-MS Neg	5533	279.3	60-33-3;	5280450	C01595
Linolenate (18:3n3 or 3n6)	0.71	4.13	0.60	Lipid	Essential fatty acid	LC-MS Neg	5450	277.3			C06427
Mevalonate*	0.55	0.99	0.17	Lipid	Mevalonate metabolism	GC-MS	1562	247	96949-03-0;	439230	C02104
Mevalonolactone	0.89	0.54	0.82	Lipid	Mevalonate metabolism	LC-MS Pos	1784	131.1	674-26-0;	10428	
myo-Inositol	1.01	0.69	0.16	Lipid	Inositol metabolism	GC-MS	1924.9	217	87-89-8;		C00137
Myristate (14:0)	2.30	1.70	0.18	Lipid	Long-chain fatty acid	LC-MS Neg	5439	227.3	544-63-8;	11005	C06424
Myristoleate (14:1n5)	0.77	6.14	0.49	Lipid	Long-chain fatty acid	LC-MS Neg	5338	225.3	544-64-9;	5281119	C08322
Oleate (18:1n9)	0.91	2.28	3.23	Lipid	Long-chain fatty acid	GC-MS	1984.4	339.2	112-80-1;	445639	C00712
Palmitate (16:0)	0.87	1.71	0.45	Lipid	Long-chain fatty acid	LC-MS Neg	5619	255.3	57-10-3;	985	C00249
Palmitoleate (16:1n7)	0.80	3.21	0.70	Lipid	Long-chain fatty acid	LC-MS Neg	5477	253.3	373-49-9;	445638	C08362
Palmitoyl ethanolamide	0.86	0.67	2.24	Lipid	Endocannabinoid	LC-MS Pos	5742	300.4		4671	
Phytosphingosine	1.37	0.14	0.78	Lipid	Sphingolipid	LC-MS Pos	5189	318.4	554-62-1;		C12144
scyllo-Inositol	0.94	0.80	0.96	Lipid	Inositol metabolism	GC-MS	1893.8	318.2	488-59-5;		C06153
Sphinganine	1.15	0.36	0.79	Lipid	Sphingolipid	LC-MS Pos	5175	302.3	3102-56-5;	3126	C00836
Sphingosine	1.40	0.39	0.85	Lipid	Sphingolipid	LC-MS Pos	5197	300.2	123-78-4;	5353955	C00319
Squalene	0.97	0.46	1.02	Lipid	Sterol-steroid	GC-MS	2205	69	111-02-4;	638072	C00751
Stearate (18:0)	0.88	1.53	0.52	Lipid	Long-chain fatty acid	LC-MS Neg	5886	283.4	57-11-4;	5281	C01530
Taurocholate	0.40	1.57	3.72	Lipid	Bile acid metabolism	LC-MS Neg	5122	514.3	145-42-6;		C05122
Undecanedioate	1.04	1.08	0.33	Lipid	Fatty acid, dicarboxylate	LC-MS Neg	2376	215.1	1852-04-6;	15816	
2'-Deoxyadenosine	1.75	0.43	0.25	Nucleotide	Purine metabolism, adenine containing	LC-MS Pos	1632	252.1	16373-93-6;	13730	C00559
2'-O-Methylguanosine	2.64	0.47	0.44	Nucleotide	Purine metabolism, guanine containing	LC-MS Neg	1901	296.2	2140-71-8;		C04545
5-Methyluridine (ribothymidine)	0.94	1.14	1.16	Nucleotide	Pyrimidine metabolism, uracil containing	LC-MS Neg	1774	257.1	1463-10-1;	445408	
7-Methylguanine	2.81	0.26	0.30	Nucleotide	Purine metabolism, guanine containing	GC-MS	1968	294	578-76-7;	11361	C02242

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	Concentration								Identifier		
Compound	Day 4	Day 9	Day 15	Super pathway	Subpathway	Platform	RI	Mass	CAS	PUBCHEM	KEGG
Adenine	0.04	1.07	1.36	Nucleotide	Purine metabolism, adenine containing	LC-MS Pos	1003	136.1	73-24-5;	190	C00147
Adenosine	0.14	2.05	0.34	Nucleotide	Purine metabolism, adenine containing	LC-MS Pos	1650	268.1	58-61-7;	60961	C00212
3'-AMP	0.51	5.51	0.56	Nucleotide	Purine metabolism, adenine containing	LC-MS Neg	1268	346.1	84-21-9;	15938966	C01367
Amp	1.37	0.86	0.01	Nucleotide	Purine metabolism, adenine containing	LC-MS Pos	1210	348.1	149022-20-8;	15938965	C00020
Adenylosuccinate	0.98	1.20	0.08	Nucleotide	Purine metabolism, adenine containing	LC-MS Neg	569	462.1	19046-78-7;	195	C03794
Cytidine	0.07	0.95	1.22	Nucleotide	Pyrimidine metabolism, cytidine containing	LC-MS Pos	1065	244	65-46-3;	6175	C00475
CMP	0.57	1.12	0.16	Nucleotide	Pyrimidine metabolism, cytidine containing	LC-MS Pos	887	324	63-37-6;	7058165	C00055
Guanine	1.03	0.82	1.48	Nucleotide	Purine metabolism, guanine containing	GC-MS	1942.3	352.1	73-40-5;	764	C00242
Guanosine	0.11	1.73	0.54	Nucleotide	Purine metabolism, guanine containing	LC-MS Pos	1676	284	118-00-3;	6802	C00387
Guanosine-2',3'-cyclic monophosphate	0.24	4.23	2.45	Nucleotide	Purine metabolism, guanine containing	LC-MS Neg	1454	343.9		417655	C06194
Hypoxanthine	6.16	0.76	0.12	Nucleotide	Purine metabolism, (hypo)xanthine-inosine containing	GC-MS	1759.2	265	68-94-0;	790	C00262
Inosine	1.01	1.10	0.05	Nucleotide	Purine metabolism, (hypo)xanthine-inosine containing	LC-MS Neg	1630	267.2	58-63-9;		
Methylphosphate	3.35	0.86	0.45	Nucleotide	Purine and pyrimidine metabolism	GC-MS	1221	240.9	7023-27-0;	13130	
Pseudouridine	4.09	0.60	0.23	Nucleotide	Pyrimidine metabolism, uracil containing	LC-MS Neg	1104	243.1	1445-07-4;		C02067
Thymidine	3.43	0.45	0.38	Nucleotide	Pyrimidine metabolism, thymine containing	LC-MS Pos	1976	242.9	50-89-5;	5789	C00214
Uracil	17.43	0.18	0.10	Nucleotide	Pyrimidine metabolism, uracil containing	GC-MS	1370.4	241	66-22-8;	1174	C00106
Urate	0.84	1.03	1.37	Nucleotide	Purine metabolism, urate metabolism	GC-MS	1928	441.2	69-93-2;120K5305;		C00366
Uridine	0.21	1.41	0.63	Nucleotide	Pyrimidine metabolism, uracil containing	LC-MS Neg	1467	243.1	58-96-8;	6029	C00299
Uridine monophosphate (5' or 3')	0.67	1.65	0.12	Nucleotide	Pyrimidine metabolism, uracil containing	LC-MS Pos	1079	325			

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	Concentration								Identifier		
Compound	Day 4	Day 9	Day 15	Super pathway	Subpathway	Platform	RI	Mass	CAS	PUBCHEM	KEGG
Xanthine	16.56	0.46	0.39	Nucleotide	Purine metabolism, (hypo)xanthine/ inosine containing	GC-MS	1889.9	353	69-89-6;	1188	C00385
Alanylleucine	0.80	3.14	0.85	Peptide	Dipeptide	LC-MS Pos	2150	203		259583	
Aspartylleucine	0.71	3.01	0.90	Peptide	Dipeptide	LC-MS Pos	2310	247.2	3062-14-4;	332962	
Aspartylphenylalanine	1.04	1.53	0.85	Peptide	Dipeptide	LC-MS Pos	2538	281.1	13433-09-5;	93078	
g-Glutamyl-2-aminobutyrate	11.14	0.87	0.24	Peptide	Gamma-glutamyl	LC-MS Pos	1589	233.1			
g-Glutamylcysteine	2.40	1.08	0.09	Peptide	Gamma-glutamyl	LC-MS Pos	1274	251.1	636-58-8;	842	C00669
g-Glutamylglycine	1.55	0.81	0.09	Peptide	Gamma-glutamyl	GC-MS	1934	375.2	1948-29-4;	165527	
g-Glutamylisoleucine	1.08	0.41	0.55	Peptide	Gamma-glutamyl	LC-MS Pos	2644	261.2			
g-Glutamylleucine	2.88	0.50	0.51	Peptide	Gamma-glutamyl	LC-MS Pos	2744	261.2	2566-39-4;	151023	
g-Glutamylphenylalanine	1.39	0.72	1.10	Peptide	Gamma-glutamyl	LC-MS Pos	2846	295.1	7432-24-8;	111299	
Glycylisoleucine	2.32	0.88	0.43	Peptide	Dipeptide	LC-MS Pos	2080	189.1	19461-38-2;		
Glycylleucine	4.16	1.09	0.23	Peptide	Dipeptide	LC-MS Pos	2236	189.1	869-19-2;	928,431,548,899	C02155
Glycylproline	8.82	0.51	0.28	Peptide	Dipeptide	LC-MS Pos	1115	173.1	704-15-4;	30,136,256, 993,386	
Isoleucylalanine	0.83	1.55	1.01	Peptide	Dipeptide	LC-MS Pos	1686	203.2	24787-73-3;	52,460,095, 246,010	
Isoleucylglycine	2.86	0.72	0.76	Peptide	Dipeptide	LC-MS Pos	1732	189.2	868-28-0;	342532	
Isoleucylisoleucine	1.06	1.24	0.41	Peptide	Dipeptide	LC-MS Pos	2678	245.1	42537-99-5;		
Isoleucylleucine	0.55	1.39	1.38	Peptide	Dipeptide	LC-MS Pos	2856	245.1	26462-22-6;	11644431	
Leucylalanine	0.99	0.87	1.24	Peptide	Dipeptide	LC-MS Pos	1760	203.2	7298-84-2;	259321	
Leucylglycine	0.70	0.97	2.03	Peptide	Dipeptide	LC-MS Pos	1800	189.2	686-50-0;	79070	
Leucylleucine	1.16	0.93	3.27	Peptide	Dipeptide	LC-MS Pos	3012	245.1	3303-31-9;	768,076, 992,072	C11332
Leucylmethionine	0.67	1.76	1.45	Peptide	Dipeptide	LC-MS Pos	2504	263.2	36077-39-1;	118276	
Phenylalanylisoleucine	0.16	1.45	0.78	Peptide	Dipeptide	LC-MS Neg	4129	277.3	22951-94-6;		
Phenylalanylleucine	0.26	1.22	1.77	Peptide	Dipeptide	LC-MS Pos	3273	279.2	3303-55-7;	4078229	
Pro-Pro-Pro	1.04	0.27	0.01	Peptide	Polypeptide	LC-MS Pos	1720.1	310.2	19285-44-0;	4475718	
Serylleucine	0.75	1.91	0.31	Peptide	Dipeptide	LC-MS Pos	2106	219.2	6665-16-3;		
Serylphenyalanine	0.81	1.59	0.79	Peptide	Dipeptide	LC-MS Pos	2348	253.2			
Threonylleucine	0.71	3.08	0.71	Peptide	Dipeptide	LC-MS Pos	2204	233.2	50299-12-2;	4420322	
Threonylphenylalanine	0.31	2.18	0.48	Peptide	Dipeptide	LC-MS Pos	2500	267.2		40,997,994, 099,798	
Tyrosylisoleucine	0.35	1.51	1.45	Peptide	Dipeptide	LC-MS Pos	2518	295.2	40829-32-1;		
Tyrosylleucine	0.59	1.80	1.47	Peptide	Dipeptide	LC-MS Pos	2656	295.2	17355-10-1;	870,717,009,561	

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	Concentration								Identifier		
Compound	Day 4	Day 9	Day 15	Super pathway	Subpathway	Platform	RI	Mass	CAS	PUBCHEM	KEGG
2,4,6-Trihydroxybenzoate	0.99	2.03	1.13	Xenobiotics	Benzoate metabolism	LC-MS Neg	1571	169.1	83-30-7;	66520	
2-(3,4-Dihydroxyphenyl)-3,5,7-Trihydroxy-4-chromanone	0.49	1.70	4.53	Xenobiotics	Food component/plant	LC-MS Neg	2210	303.2	480-18-2;	471	
2-Pyrrolidinone	0.76	1.47	0.30	Xenobiotics	Chemical	GC-MS	1190.9	142	616-45-5;	12025	
3,4-Dihydroxybenzoate	0.87	1.40	1.35	Xenobiotics	Benzoate metabolism	GC-MS	1768	193	99-50-3;	72	C00230
3,4-Dihydroxyphenylethanol	1.71	0.83	0.99	Xenobiotics	Food component/plant	GC-MS	1727	267.1	10597-60-1;		
3-Deoxyoctulosonate	1.22	0.79	0.83	Xenobiotics	Bacterial	GC-MS	1942	373.2	103404-70-2;	4636210	
Caffeate	0.37	1.16	2.49	Xenobiotics	Food component/plant	GC-MS	1949.9	396.2	331-39-5;	689043	C01197
Dihydrokaempferol	0.53	1.50	3.58	Xenobiotics	Food component/plant	LC-MS Neg	2568	287	480-20-6;		C00974
Erythritol	2.37	1.21	0.52	Xenobiotics	Sugar, sugar substitute, starch	GC-MS	1517.5	217	149-32-6;		C00503
Galactarate (mucic acid)	0.79	1.12	1.97	Xenobiotics	Sugar, sugar substitute, starch	GC-MS	1899.3	333.1	526-99-8;	3037582	C00879
Galactonate	0.26	1.91	0.51	Xenobiotics	Food component/plant	GC-MS	1813.6	217.1	299-28-5;	128869	C00880
Galacturonate	0.51	1.14	1.49	Xenobiotics	Sugar, sugar substitute, starch	GC-MS	1888.7	204	91510-62-2;	84740	C08348
Gallate	0.70	1.00	1.10	Xenobiotics	Food component/plant	GC-MS	1857	281	149-91-7;	370	D01398,C01424
Glycerol 2-phosphate	1.10	0.78	0.06	Xenobiotics	Chemical	GC-MS	1691.8	243	819-83-0;	2526	C02979,D01488
Glycolate (hydroxyacetate)	1.12	0.58	0.29	Xenobiotics	Chemical	GC-MS	1119	177	79-14-1;	3,698,251,757	C00160
Isorhamnetin	0.87	0.79	4.96	Xenobiotics	Food component/plant	LC-MS Neg	4086.8	315.1	480-19-3;	5281654	C10084
Kaempferol	0.86	1.11	2.43	Xenobiotics	Food component/plant	LC-MS Pos	4587	287.1	520;	5280863	C05903
Kaempferol 3-*O*-beta-glucoside	0.46	1.47	2.51	Xenobiotics	Food component/plant	LC-MS Pos	3884	449	480-10-4;		
Lidocaine	0.31	0.74	13.16	Xenobiotics	Drug	LC-MS Pos	2761	235.2	137-58-6;	3676	D00358
Naringenin	0.56	1.52	2.75	Xenobiotics	Food component-plant	LC-MS Neg	3484	271.1	67604-48-2;	932	C00509
p-Aminobenzoate (PABA)	0.77	0.58	0.25	Xenobiotics	Benzoate metabolism	LC-MS Pos	2120	138.1	150-13-0;	7,057,990,978	C00568
Quercetin	0.21	1.20	2.82	Xenobiotics	Food component/plant	LC-MS Pos	4262	303.1	849061-97-8;	5280343	C00389
Quercetin-3-galactoside	0.34	1.60	2.99	Xenobiotics	Food component/plant	LC-MS Neg	2706	463.2	482-36-0;	5281643	C10073
Quinate	1.01	0.86	1.00	Xenobiotics	Food component/plant	GC-MS	1791.5	345.1	77-95-2;		C00296
Shikimate	0.72	1.23	1.39	Xenobiotics	Food component/plant	GC-MS	1758.1	204	138-59-0;	8742	C00493
Tartarate	0.83	1.12	3.56	Xenobiotics	Food component/plant	LC-MS Neg	604	149.1	6106-24-7;	875	C00898
Trehalose 6-phosphate	0.13	2.20	0.05	Xenobiotics	Sugar, sugar substitute, starch	GC-MS	2310	315.16	136632-28-5;	122336	C00689
Trihydroxybutane	1.28	0.39	0.18	Xenobiotics	Food component/plant	GC-MS	1329.5	117	4435-50-1;	20497	
Quercetin-3-*O*-glucoside	0.41	1.56	2.96			LC-MS Neg	2770	463	21637-25-2;		
X – 03002	5.02	0.67	0.45			GC-MS	1438.1	296.1			
X – 03094	3.65	0.85	0.67			GC-MS	1978.7	299			
X – 03998	1.65	0.38	0.36			GC-MS	1252	171			
X – 04006	2.26	0.42	0.39			GC-MS	1409.4	102			

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	Concentration								Identifier		
Compound	Day 4	Day 9	Day 15	Super pathway	Subpathway	Platform	RI	Mass	CAS	PUBCHEM	KEGG
X – 04033	3.93	1.11	0.17			GC-MS	1774.6	112			
X – 04051	2.02	0.78	0.98			GC-MS	1968.7	357.1			
X – 05214	0.41	1.47	0.49			GC-MS	1960	117			
X – 05228	1.83	0.30	0.29			GC-MS	1442.5	181.1			
X – 05406	0.99	0.87	0.75			GC-MS	1404.6	306			
X – 06650	1.33	1.49	0.21			GC-MS	1991.9	188.2			
X – 06666	1.79	0.93	0.22			GC-MS	2053.1	318.2			
X – 06667	0.78	1.12	0.75			GC-MS	2074	217.1			
X – 08889	0.94	7.70	0.11			GC-MS	1634.3	521.2			
X – 08895	4.35	0.56	0.14			GC-MS	1792.3	174.1			
X – 09429	3.02	0.06	0.04			GC-MS	2286.3	204			
X – 10356	1.76	0.98	0.25			GC-MS	1714.4	333			
X – 10358	1.25	0.96	0.54			GC-MS	1729.5	292.1			
X – 10500	1.14	0.83	0.30			GC-MS	1229.9	211			
X – 10607	1.61	1.21	0.14			GC-MS	1918	326.1			
X – 10649	2.08	1.07	0.71			GC-MS	1345.7	140			
X – 10677	1.88	0.93	0.17			GC-MS	1438	269.1			
X – 10806	0.16	1.88	1.33			GC-MS	2189	318.2			
X – 10876	1.86	0.92	0.37			GC-MS	1485.9	70.9			
X – 10882	1.20	0.23	0.17			GC-MS	1774	367.1			
X – 11334	0.44	1.32	0.46			LC-MS Pos	982	259.1			
X – 11583	1.06	0.95	0.08			LC-MS Pos	2793	457.1			
X – 11585	0.92	1.93	0.61			LC-MS Pos	2987	332			
X – 11586	1.27	0.39	0.11			LC-MS Pos	3434	442			
X – 11587	1.11	0.36	0.36			LC-MS Pos	3502	485.1			
X – 11624	2.60	0.45	0.18			LC-MS Pos	2727.9	279			
X – 11687	3.65	0.42	0.40			LC-MS Pos	2182	384.1			
X – 11755	0.81	1.23	0.90			GC-MS	1820	318.2			
X – 11795	19.76	2.25	0.52			LC-MS Pos	1457	148.1			
X – 12051	51.63	0.84	0.33			LC-MS Pos	5739	456.4			
X – 12100	1.13	0.81	1.13			LC-MS Pos	1793	221.1			
X – 12259	0.65	0.89	1.94			LC-MS Neg	724	133.2			
X – 12421	1.59	0.75	0.75			LC-MS Pos	5876	370			
X – 12422	1.54	0.69	0.69			LC-MS Pos	5937	370			

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	Concentration								Identifier		
Compound	Day 4	Day 9	Day 15	Super pathway	Subpathway	Platform	RI	Mass	CAS	PUBCHEM	KEGG
X – 12462	1.05	0.44	0.61			LC-MS Pos	1269	148.2			
X – 12510	0.96	0.88	0.88			LC-MS Pos	3343	160.2			
X – 12602	0.48	0.36	0.12			LC-MS Pos	1456	204.2			
X – 12660	1.39	0.66	0.66			LC-MS Pos	5667	442.2			
X – 12689	0.83	1.07	0.23			LC-MS Pos	1183	278.2			
X – 12824	1.03	1.97	0.42			LC-MS Neg	2803	243.2			
X – 12874	1.03	0.77	0.24			LC-MS Neg	4714	231.2			
X – 12886	0.93	0.88	1.10			LC-MS Neg	1007	189.2			
X – 12948	11.74	0.79	0.35			LC-MS Pos	1815	350.1			
X – 13042	0.96	0.93	1.18			LC-MS Neg	3193	385.2			
X – 13046	0.87	1.12	2.60			LC-MS Neg	1459	315.2			
X – 13111	0.68	1.69	0.69			LC-MS Pos	1386	344.2			
X – 13230	0.84	1.02	0.99			LC-MS Neg	674	161			
X – 13496	0.67	1.43	1.21			GC-MS	2103.4	372.2			
X – 13497	1.01	0.88	0.10			GC-MS	1596	211			
X – 13502	2.25	0.66	0.09			LC-MS Pos	874	306.1			
X – 13746	0.74	0.97	0.32			GC-MS	1956	217.1			
X – 13772	0.87	2.08	0.63			LC-MS Neg	1799	243.2			
X – 13875	1.19	0.81	1.06			LC-MS Neg	1773	251.1			
X – 13928	0.89	0.32	0.38			LC-MS Pos	1947	190.1			
X – 14150	0.86	1.80	0.19			LC-MS Pos	1592	219.2			
X – 14294	0.13	0.20	2.03			LC-MS Neg	2186	422.2			
X – 14306	0.22	1.31	2.85			LC-MS Pos	2463	359.3			
X – 14338	0.41	2.09	2.14			LC-MS Pos	2600	265.2			
X – 14564	1.09	0.89	0.79			LC-MS Neg	6161	345.4			
X – 14900	0.86	1.05	1.31			LC-MS Neg	2117	258.2			
X – 15124	1.86	0.27	0.20			LC-MS Pos	1776	300			
X – 15134	1.91	0.44	0.31			LC-MS Pos	3198	321.1			
X – 15136	1.50	0.93	0.14			LC-MS Pos	4063	243.1			
X – 15312	1.03	1.25	0.41			LC-MS Pos	3079	331.9			
X – 15375	0.56	0.89	0.37			LC-MS Pos	2502	328			
X – 15382	1.28	0.69	0.63			LC-MS Pos	2540	271			
X – 15421	0.33	0.64	4.77			LC-MS Neg	3307	490.1			
X – 15422	4.65	0.98	0.32			LC-MS Neg	922	199			

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	Concentration								Identifier		
Compound	Day 4	Day 9	Day 15	Super pathway	Subpathway	Platform	RI	Mass	CAS	PUBCHEM	KEGG
X – 15484	1.66	0.78	0.86			LC-MS Pos	2506	271			
X – 15516	1.80	0.57	0.38			LC-MS Pos	1718	246.1			
X – 15532	1.04	0.96	0.29			LC-MS Pos	2351	260.2			
X – 15537	1.44	0.88	0.41			LC-MS Pos	4211	192.1			
X – 15546	3.84	0.69	0.29			LC-MS Pos	1861	271.1			
X – 15558	0.70	0.76	0.35			LC-MS Pos	4346	342.1			
X – 15562	0.86	1.28	0.12			LC-MS Pos	4686	470.1			
X – 15563	0.78	1.31	0.11			LC-MS Pos	4749	490			
X – 15591	0.77	0.62	0.06			LC-MS Neg	1790	203.1			
X – 15787	0.97	1.27	0.09			GC-MS	2103	519.4			
X – 15797	1.63	0.19	0.26			LC-MS Neg	1786	160.2			
X – 15807	2.89	0.17	0.17			LC-MS Neg	3366	337.2			
X – 15812	2.03	0.82	0.15			LC-MS Pos	1716	375.1			
X – 15819	0.14	0.74	0.14			GC-MS	2066	315.1			
X – 15868	0.94	1.00	1.73			LC-MS Neg	1516	325.1			
X – 16063	3.83	0.65	0.32			LC-MS Neg	4770	341.1			
X – 16094	1.12	0.12	0.08			LC-MS Pos	3691	276.2			
X – 16296	0.88	0.98	1.50			LC-MS Neg	3463.6	174.1			
X – 16310	0.32	1.43	0.54			LC-MS Pos	924.7	212.1			
X – 16439	0.67	1.10	0.36			LC-MS Pos	3795.8	322.1			
X – 16468	1.20	0.85	0.30			LC-MS Pos	2143.4	246.1			
X – 16693	1.19	0.80	0.23			LC-MS Pos	1628.4	176			
X – 16869	0.97	0.03	0.03			LC-MS Neg	5179.8	330.2			
X – 17071	10.22	0.34	0.27			LC-MS Neg	2058.5	399.1			
X – 17147	1.89	1.04	0.35			LC-MS Neg	4830	187.2			
X – 17151	1.48	0.72	0.54			LC-MS Neg	4811	169.2			
X – 17430	0.83	1.26	0.23			LC-MS Pos	4716.8	473.3			
X – 17485	2.42	1.10	0.05			GC-MS	2031	493.2			
X – 17491	6.05	1.05	0.05			LC-MS Neg	1188.9	405.2			
X – 17543	1.03	0.25	0.29			LC-MS Neg	1236.4	188.2			

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	Concentration								Identifier		
Compound	Day 4	Day 9	Day 15	Super pathway	Subpathway	Platform	RI	Mass	CAS	PUBCHEM	KEGG
3-(4-Hydroxyphenyl)lactate (HPLA)	0.76	1.24	0.95	Amino acid	Phenylalanine and tyrosine metabolism	LC-MS Neg	1395	181.1	6482-98-0;	9378	C03672
4-Guanidinobutanoate	1.88	1.26	0.89	Amino acid	Guanidino and acetamido metabolism	LC-MS Pos	1085	146.1	463-003;463-00-3;	500	C01035
5-Oxoproline	1.02	1.04	1.12	Amino acid	Glutathione metabolism	LC-MS Pos	1446	130.1	98-79-3;	7405	C01879
Agmatine	0.18	0.98	0.98	Amino acid	Polyamine metabolism	GC-MS	1526	174	2482-00-0;	199	C00179
Alanine	1.11	1.29	2.95	Amino acid	Alanine and aspartate metabolism	GC-MS	1147.6	115.9	56-41-7;	59,507,311,724	C00041
allo-threonine	0.93	0.95	0.94	Amino acid	Glycine, serine, and threonine metabolism	GC-MS	1417.8	219	28954-12-3;	992,896,995,276	C05519
a-Hydroxyisovalerate	0.97	1.07	0.72	Amino acid	Valine, leucine, and isoleucine metabolism	GC-MS	1208	145.1	600-37-3;	99823	
Arginine	1.99	0.87	1.12	Amino acid	Urea cycle; arginine and proline metabolism	LC-MS Pos	650	175.2	1119-34-2;	5,246,487,232	C00062
Asparagine	0.46	1.73	2.28	Amino acid	Alanine and aspartate metabolism	GC-MS	1651.2	231	70-47-3;	62,676,992,089	C00152
Aspartate	0.43	1.22	3.61	Amino acid	Alanine and aspartate metabolism	GC-MS	1529.7	232	56-84-8;	5960	C00049
b-Alanine	1.21	1.03	1.16	Amino acid	Alanine and aspartate metabolism	GC-MS	1451.8	174	56-41-7;107-95-9;	2,394,755,801	C00099
b-Hydroxypyruvate	3.16	1.33	0.90	Amino acid	Glycine, serine, and threonine metabolism	GC-MS	1425.1	221	3369-79-7;	964	C00168
Betaine	0.27	0.75	1.43	Amino acid	Glycine, serine, and threonine metabolism	LC-MS Pos	721	118.2	107-43-7;	247	
Citramalate	0.79	1.81	1.87	Amino acid	Valine, leucine, and isoleucine metabolism	GC-MS	1490.7	247	6236-10-8;	1081	C02612,C00815
g-Aminobutyrate (GABA)	1.11	1.24	1.21	Amino acid	Glutamate metabolism	GC-MS	1539.7	304.1	56-12-2;	6,992,099,119	C00334
Glutamate	1.64	1.03	2.49	Amino acid	Glutamate metabolism	GC-MS	1611.9	246	56-86-0;	611	C00025
Glutamine	0.88	0.99	1.14	Amino acid	Glutamate metabolism	LC-MS Pos	684	147.2	56-85-9;	69,920,865,961	C00064
Glutarate (pentanedioate)	0.47	1.08	1.27	Amino acid	Lysine metabolism	GC-MS	1433.6	261	110-94-1;	4418048	C00489
Glutathione, oxidized (GSSG)	0.74	1.03	1.56	Amino acid	Glutathione metabolism	LC-MS Pos	1535	613.1	103239-24-3;	6,535,911,215,652	C00127
Glutathione, reduced (GSH)	0.27	3.83	3.65	Amino acid	Glutathione metabolism	LC-MS Pos	1274	308.1	70-18-8;	124886	C00051
Glycine	0.39	1.27	1.71	Amino acid	Glycine, serine, and threonine metabolism	GC-MS	1166	101.9	56-40-6;	5,257,127,750	C00037
Histidine	1.51	1.82	3.71	Amino acid	Histidine metabolism	GC-MS	1837.3	154	5934-29-2;	7,733,651,426	C00135
Homoserine (homoserine lactone)	0.89	1.57	3.35	Amino acid	Glycine, serine, and threonine metabolism	GC-MS	1471	218.1	672-15-1;	126,476,971,022	C00263,C02926
Imidazole lactate	1.21	1.07	0.93	Amino acid	Histidine metabolism	LC-MS Pos	778	157.1	14403-45-3;	440129	C05568
Isoleucine	0.46	1.49	4.80	Amino acid	Valine, leucine, and isoleucine metabolism	LC-MS Pos	1614	132.1	73-32-5;	791	C00407

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Compound	Day 4	Day 9	Day 15	Super pathway	Subpathway	Platform	RI	Mass	CAS	PUBCHEM	KEGG
Kynurenate	1.31	1.11	0.73	Amino acid	Tryptophan metabolism	LC-MS Neg	2243	188.1	492-27-3;	3845	C01717
Kynurenine	1.31	0.93	0.76	Amino acid	Tryptophan metabolism	LC-MS Pos	1902	209.1	2922-83-0;	1,611,666,971,029	C00328
Leucine	0.22	1.24	5.74	Amino acid	Valine, leucine, and isoleucine metabolism	LC-MS Pos	1674	132.2	61-90-5;	70,457,986,106	C00123
Lysine	0.37	1.08	4.40	Amino acid	Lysine metabolism	GC-MS	1836.7	317.2	56-87-1;	5962	C00047
Methionine	0.99	1.65	2.37	Amino acid	Cysteine, methionine, SAM, taurine metabolism	LC-MS Pos	1252	150.1	63-68-3;	69,920,876,137	C00073
N-Acetylglutamine	1.03	0.99	1.15	Amino acid	Glutamate metabolism	LC-MS Pos	1204	189.1	2490-97-3;	182230	C02716
N-Acetylglycine	0.46	1.03	1.55	Amino acid	Glycine, serine, and threonine metabolism	GC-MS	1396.4	143.9	543-24-8;	10972	
N-Acetylisoleucine	1.05	1.34	0.90	Amino acid	Valine, leucine, and isoleucine metabolism	LC-MS Pos	3370	174.1		2802421	
N-Acetylleucine	0.55	1.82	1.28	Amino acid	Valine, leucine, and isoleucine metabolism	LC-MS Pos	3444	174.1	1188-21-2;	70912	C02710
N-Acetylmethionine	0.72	1.13	1.57	Amino acid	Cysteine, methionine, SAM, taurine metabolism	LC-MS Neg	1805	190.1	65-82-7;	448580	C02712
N-Acetylphenylalanine	0.51	1.21	1.11	Amino acid	Phenylalanine and tyrosine metabolism	LC-MS Pos	3563	208.1	2018-61-3;	74839	C03519
N-Acetylproline	0.54	2.89	3.37	Amino acid	Urea cycle; arginine and proline metabolism	LC-MS Pos	2184	158.1	1074-79-9;	322640	
N-Acetylvaline	0.59	1.02	1.32	Amino acid	Valine, leucine, and isoleucine metabolism	LC-MS Pos	2654	160.1	96-81-1;	66789	
N_6-acetyllysine	0.69	1.02	1.48	Amino acid	Lysine metabolism	LC-MS Pos	1134	189.1	692-04-6;	699,197,892,832	C02727
Phenethylamine (isobar with 1-phenylethanamine)	1.05	1.09	1.00	Amino acid	Phenylalanine and tyrosine metabolism	LC-MS Pos	2114.7	122.1			C02455, C05332
Phenylalanine	0.19	1.15	4.74	Amino acid	Phenylalanine and tyrosine metabolism	LC-MS Pos	2056	166.1	63-91-2;	69,256,656,140	C00079
Phenyllactate (PLA)	0.23	0.98	0.87	Amino acid	Phenylalanine and tyrosine metabolism	LC-MS Neg	2237	165.1	828-01-3;	3848	C05607
Pipecolate	0.79	1.04	1.08	Amino acid	Lysine metabolism	GC-MS	1396.1	156	4043-87-2;	849	C00408
Proline	0.84	0.97	1.07	Amino acid	Urea cycle; arginine and proline metabolism	LC-MS Pos	796	116.1	147-85-3;	1,457,426,971,047	C00148
Putrescine	1.15	1.25	1.47	Amino acid	Polyamine metabolism	GC-MS	1705.8	174	110-60-1;		C00134
Pyroglutamine	0.92	0.97	1.01	Amino acid	Glutamate metabolism	LC-MS Pos	764	129.2		134508	
S-Adenosylhomocysteine (SAH)	1.04	1.05	1.00	Amino acid	Cysteine, methionine, SAM, taurine metabolism	LC-MS Neg	1821	383.1	979-92-0;		C00021

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	Concentration								Identifier		
Compound	Day 4	Day 9	Day 15	Super pathway	Subpathway	Platform	RI	Mass	CAS	PUBCHEM	KEGG
S-Adenosylmethionine (SAM)	0.08	1.57	3.26	Amino acid	Cysteine, methionine, SAM, taurine metabolism	LC-MS Pos	676	399.1	24346-00-7;		
Saccharopine	0.17	1.12	3.49	Amino acid	Lysine metabolism	LC-MS Pos	695	277.1	997-68-2;	160556	C00449
Serine	0.59	1.58	3.00	Amino acid	Glycine, serine, and threonine metabolism	GC-MS	1389.1	204	56-45-1;	59,516,857,581	C00065
Spermidine	0.77	1.45	5.08	Amino acid	Polyamine metabolism	GC-MS	1998.9	144	124-20-9;	1102	C00315
Threonine	0.56	0.88	1.95	Amino acid	Glycine, serine, and threonine metabolism	LC-MS Pos	713	120.1	72-19-5;	69,710,196,288	C00188
Hydroxyproline	0.86	1.12	1.07	Amino acid	Urea cycle; arginine and proline metabolism	GC-MS	1537	140	51-35-4;	58,106,971,053	C01157
Tryptophan	3.33	0.96	0.99	Amino acid	Tryptophan metabolism	LC-MS Pos	2445	205.1	73-22-3;	69,235,166,305	C00078
Tyrosine	1.66	0.99	1.81	Amino acid	Phenylalanine and tyrosine metabolism	LC-MS Pos	1516	182.1	60-18-4;	60,576,942,100	C00082
Urea	0.19	0.90	1.35	Amino acid	Urea cycle; arginine and proline metabolism	GC-MS	1287.7	189	57-13-6;	117,616,150,869	C00086
Valine	0.60	1.11	4.48	Amino acid	Valine, leucine, and isoleucine metabolism	LC-MS Pos	1040	118.1	72-18-4;	69,710,186,287	C00183
Dihydroxyacetone	21.27	2.28	0.32	Carbohydrate	Glycolysis, gluconeogenesis, pyruvate metabolism	GC-MS	1263	103	62147-49-3;	670	C00184
2,3-Butanediol	0.78	2.15	1.50	Carbohydrate	Glycolysis, gluconeogenesis, pyruvate metabolism	GC-MS	1075	116.9	24347-58-8;		C03044
2-Isopropylmalate	0.73	0.70	0.66	Carbohydrate	Glycolysis, gluconeogenesis, pyruvate metabolism	LC-MS Pos	2917	194.1	3237-44-3;	77	C02504
Arabinose	0.78	1.10	1.10	Carbohydrate	Nucleotide sugars, pentose metabolism	GC-MS	1631.6	217	28697-53-2;	66308	C00181
Arabitol	0.83	0.98	1.04	Carbohydrate	Nucleotide sugars, pentose metabolism	GC-MS	1687.5	307.1	488-82-4;	94154	C00474
Erythronate	0.81	1.17	1.08	Carbohydrate	Amino-sugar metabolism	GC-MS	1546.9	292.1	13752-84-6;	2781043	
Erythrose	2.41	1.69	0.56	Carbohydrate	Fructose, mannose, galactose, starch, and sucrose metabolism	GC-MS	1431.1	217.1	583-50-6;	94176	C01796
Fructose	1.75	1.28	0.04	Carbohydrate	Fructose, mannose, galactose, starch, and sucrose metabolism	GC-MS	1758	217	57-48-7;	5984	C00095
Fructose 6-phosphate	2.29	1.28	0.73	Carbohydrate	Glycolysis, gluconeogenesis, pyruvate metabolism	GC-MS	1994.9	315.1	103213-47-4;		C05345
Galactinol	1.51	1.17	0.72	Carbohydrate	Fructose, mannose, galactose, starch, and sucrose metabolism	GC-MS	2226.1	433.3	16908-86-4;		C01235

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Compound	Day 4	Day 9	Day 15	Super pathway	Subpathway	Platform	RI	Mass	CAS	PUBCHEM	KEGG
Galactitol (dulcitol)	0.66	0.96	1.18	Carbohydrate	Fructose, mannose, galactose, starch, and sucrose metabolism	GC-MS	1849.2	319.1	608-66-2;	11850	C01697
Galactose	21.85	1.36	0.69	Carbohydrate	Fructose, mannose, galactose, starch, and sucrose metabolism	GC-MS	1793.8	203.9	59-23-4;	3037556	C01582
Glucose	15.42	2.61	0.01	Carbohydrate	Glycolysis, gluconeogenesis, pyruvate metabolism	GC-MS	1866.8	217.1	50-99-7;	79025	C00293
Glycerate	0.93	1.25	1.12	Carbohydrate	Glycolysis, gluconeogenesis, pyruvate metabolism	GC-MS	1360.7	189	600-19-1;	752	C00258
Isomaltose	0.85	1.02	1.08	Carbohydrate	Fructose, mannose, galactose, starch, and sucrose metabolism	GC-MS	2221.8	204.1	499-40-1;	439193	C00252
Lactate	1.10	1.71	0.89	Carbohydrate	Glycolysis, gluconeogenesis, pyruvate metabolism	GC-MS	1102.8	116.9	79-33-4;	612	C00186
Maltose	1.20	1.24	0.71	Carbohydrate	Fructose, mannose, galactose, starch, and sucrose metabolism	GC-MS	2142.1	204.1	6363-53-7;	439341	C00208
Mannitol	0.89	1.10	1.93	Carbohydrate	Fructose, mannose, galactose, starch, and sucrose metabolism	GC-MS	1839	319.1	69-65-8;	6251	C00392
N-Acetylglucosamine	0.73	0.79	1.01	Carbohydrate	Amino-sugar metabolism	GC-MS	1903.3	245	7512-17-6;	24139	C00140
Pyruvate	5.17	1.30	0.26	Carbohydrate	Glycolysis, gluconeogenesis, pyruvate metabolism	GC-MS	1130.6	217	127-17-3;	107735	C00022
Ribitol	0.77	0.80	0.97	Carbohydrate	Nucleotide sugars, pentose metabolism	GC-MS	1692.4	217	488-81-3;		C00474
Ribose	0.62	1.05	1.05	Carbohydrate	Nucleotide sugars, pentose metabolism	GC-MS	1639.2	204	50-69-1;	5311110	C00121
Ribulose	1.85	0.97	0.83	Carbohydrate	Nucleotide sugars, pentose metabolism	GC-MS	1662	306.1	488-84-6;	79021	C00309
Sorbitol	0.60	1.06	0.66	Carbohydrate	Fructose, mannose, galactose, starch, and sucrose metabolism	GC-MS	1843	319.1	6706-59-8;	107428	C00794
Threitol	0.95	1.16	1.01	Carbohydrate	Nucleotide sugars, pentose metabolism	GC-MS	1513	217.1	2418-52-2;	169019	C16884
Xylitol	2.14	1.29	0.59	Carbohydrate	Nucleotide sugars, pentose metabolism	GC-MS	1677.6	307.2	87-99-0;	6912	C00379
Xylonate	0.84	1.53	1.40	Carbohydrate	Nucleotide sugars, pentose metabolism	GC-MS	1722	292	73686-31-7;	6602431	C00502,C05411
Xylose	0.60	1.09	1.12	Carbohydrate	Nucleotide sugars, pentose metabolism	GC-MS	1723.9	204	609-06-3;	95259	C00181
2,3-Dihydroxyisovalerate	0.25	1.06	0.94	Cofactors and vitamins	Pantothenate and CoA metabolism	GC-MS	1422	131	1756-18-9;	677	C04039

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	Concentration								Identifier		
Compound	Day 4	Day 9	Day 15	Super pathway	Subpathway	Platform	RI	Mass	CAS	PUBCHEM	KEGG
NAD^+	0.53	1.14	3.31	Cofactors and vitamins	Nicotinate and nicotinamide metabolism	LC-MS Pos	1370	664	53-84-9;	1,089,765,158, 925,290,000	C00003
Nicotinate ribonucleoside	1.39	1.58	2.06	Cofactors and vitamins	Nicotinate and nicotinamide metabolism	LC-MS Pos	1105	256	2625-49-2;	161233	
Pantothenate (vitamin B5)	1.05	0.89	0.70	Cofactors and vitamins	Pantothenate and CoA metabolism	LC-MS Pos	2218	220.1	137-08-6;	6613	C00864
Pyridoxal	0.32	1.01	1.26	Cofactors and vitamins	Pyridoxal metabolism	LC-MS Pos	1210	168.1	65-22-5;	1050	C00250
Pyridoxate	1.00	0.97	0.95	Cofactors and vitamins	Vitamin B6 metabolism	LC-MS Neg	2210	182.1	82-82-6;	6723	C00847
Riboflavin (vitamin B2)	0.53	0.87	1.90	Cofactors and vitamins	Riboflavin metabolism	LC-MS Pos	3111	377.2	83-88-5;	493570	C00255
Threonate	0.90	1.09	1.05	Cofactors and vitamins	Ascorbate and aldarate metabolism	GC-MS	1560.7	292.1	70753-61-6;	151152	C01620
Trigonelline (*N*'-methylnicotinate)	0.60	0.89	1.15	Cofactors and vitamins	Nicotinate and nicotinamide metabolism	LC-MS Pos	757	138.1	6138-41-6;	5570	
Acetylphosphate	0.21	1.07	1.53	Energy	Oxidative phosphorylation	GC-MS	1263	211	94249-01-1;	186	C00227
a-Ketoglutarate	1.88	0.99	0.76	Energy	Krebs cycle	GC-MS	1601.5	347.1	305-72-6;328-50-7;22202-68-2;	51	C00026
Citrate	0.90	0.99	1.00	Energy	Krebs cycle	LC-MS Neg	591	191.1	77-92-9;	311	C00158
Fumarate	0.93	0.94	1.32	Energy	Krebs cycle	GC-MS	1382.1	245	100-17-8;		C00122
Homocitrate	0.89	1.06	0.98	Energy	Krebs cycle	GC-MS	1836.8	287.1	3562-74-1;	439459	C01251
Isocitrate	0.86	1.09	1.01	Energy	Krebs cycle	LC-MS Pos	953	210	20226-99-7;	1198	C00311
Malate	0.96	1.10	1.01	Energy	Krebs cycle	GC-MS	1502	233	6915-15-7;	525	C00149
Phosphate	0.86	1.18	1.25	Energy	Oxidative phosphorylation	GC-MS	1307.7	298.9	7664-38-2;	1061	C00009
Succinate	0.38	0.99	0.99	Energy	Krebs cycle	GC-MS	1348	247	110-15-6;	1110	C00042
1,2-Propanediol	0.66	1.55	1.03	Lipid	Ketone bodies	GC-MS	1041	117	57-55-6;		C00717,C02912,C00583,C01506,C02917
2-Hydroxyadipate	0.69	1.01	0.68	Lipid	Fatty acid, dicarboxylate	LC-MS Pos	1703	180.1	18294-85-4;	193530	C02360
2-Hydroxyglutarate	0.50	1.05	1.01	Lipid	Fatty acid, dicarboxylate	GC-MS	1576	247	40951-21-1;	43	C02630
2-Phenylethanol	0.94	1.46	1.16	Lipid	Fatty acid, dicarboxylate	GC-MS	1272	179.14	60-12-8;	6054	C05853,D00192
3-Isopropylmalate	0.41	0.77	0.74	Lipid	Fatty acid, dicarboxylate	GC-MS	1571.7	275.2	16048-89-8;	36	
4-Hydroxybutyrate (GHB)	0.72	1.08	0.78	Lipid	Fatty acid, monohydroxy	GC-MS	1277	233.1	502-85-2;	10413	C00989
Acetylcarnitine (C2)	0.76	0.92	1.59	Lipid	Carnitine metabolism	LC-MS Pos	1203	204.2	5080-50-2;	7045767	C02571
Caprate (10:0)	0.67	1.69	1.21	Lipid	Medium-chain fatty acid	LC-MS Neg	5092	171.2	112-37-8;	2969	C01571
Carnitine	0.67	0.72	1.08	Lipid	Carnitine metabolism	LC-MS Pos	702	162.2	461-05-2;	10917	
Ethanolamine	0.56	1.32	1.19	Lipid	Glycerolipid metabolism	GC-MS	1074	102	141-43-5;		C00189
Glycerol	0.72	1.13	0.97	Lipid	Glycerolipid metabolism	GC-MS	1311	205	56-81-5;	753	C00116
Glycerol 3-phosphate (G3P)	0.47	0.97	1.47	Lipid	Glycerolipid metabolism	GC-MS	1719.7	357.1	29849-82-9;	754	C00093

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Compound	Day 4	Day 9	Day 15	Super pathway	Subpathway	Platform	RI	Mass	CAS	PUBCHEM	KEGG
Glycerophosphoethanolamine	0.47	1.19	6.80	Lipid	Glycerolipid metabolism	GC-MS	1906	357.1	33049-08-0;	123874	C01233
Glycerophosphorylcholine (GPC)	0.07	0.85	2.04	Lipid	Glycerolipid metabolism	LC-MS Pos	694	258.1	28319-77-9;	657272	C00670
Inositol 1-phosphate (I1P)	2.03	0.90	0.71	Lipid	Inositol metabolism	GC-MS	2057.8	318.1	106032-59-1;		
Inositol 2-phosphate (I2P)	2.77	1.46	0.51	Lipid	Inositol metabolism	GC-MS	2072.9	318.1			C01177
Mevalonolactone	0.75	1.00	1.00	Lipid	Mevalonate metabolism	LC-MS Pos	1784	131.1	674-26-0;	10428	
myo-Inositol	0.62	0.95	1.26	Lipid	Inositol metabolism	GC-MS	1924.9	217	87-89-8;		C00137
scyllo-Inositol	0.77	0.91	1.21	Lipid	Inositol metabolism	GC-MS	1893.8	318.2	488-59-5;		C06153
Taurocholate	0.95	0.95	0.90	Lipid	Bile acid metabolism	LC-MS Neg	5122	514.3	145-42-6;		C05122
2'-*O*-Methylguanosine	0.79	0.72	0.62	Nucleotide	Purine metabolism, guanine containing	LC-MS Pos	1926	298	2140-71-8;		C04545
5-Methyluridine (ribothymidine)	0.73	1.15	0.76	Nucleotide	Pyrimidine metabolism, uracil containing	LC-MS Neg	1774	257.1	1463-10-1;	445408	
Adenine	0.74	3.10	9.74	Nucleotide	Purine metabolism, adenine containing	LC-MS Pos	1003	136.1	73-24-5;	190	C00147
Adenosine	1.05	0.94	1.26	Nucleotide	Purine metabolism, adenine containing	LC-MS Pos	1650	268.1	58-61-7;	60961	C00212
Cytidine	0.68	1.05	2.47	Nucleotide	Pyrimidine metabolism, cytidine containing	LC-MS Pos	1065	244	65-46-3;	6175	C00475
N_6-carbamoylthreonyladenosine	1.06	0.91	0.99	Nucleotide	Purine metabolism, guanine containing	LC-MS Pos	2656	413	24719-82-2;		
Pseudouridine	0.58	0.98	1.02	Nucleotide	Pyrimidine metabolism, uracil containing	LC-MS Neg	1104	243.1	1445-07-4;		C02067
Uracil	0.27	0.90	1.08	Nucleotide	Pyrimidine metabolism, uracil containing	GC-MS	1370.4	241	66-22-8;	1174	C00106
Urate	0.49	0.99	1.22	Nucleotide	Purine metabolism, urate metabolism	GC-MS	1928	441.2	69-93-2;120K5305;		C00366
Uridine	0.14	0.80	1.13	Nucleotide	Pyrimidine metabolism, uracil containing	LC-MS Neg	1467	243.1	58-96-8;	6029	C00299
Xanthine	0.10	0.80	1.19	Nucleotide	Purine metabolism, (hypo)xanthine-inosine containing	GC-MS	1889.9	353	69-89-6;	1188	C00385
Alanylvaline	0.86	1.33	6.06	Peptide	Dipeptide	LC-MS Pos	1513	189		137276	
g-Glutamylisoleucine	0.93	0.31	0.81	Peptide	gamma-glutamyl	LC-MS Pos	2644	261.2			
g-Glutamylleucine	1.04	0.93	0.99	Peptide	gamma-glutamyl	LC-MS Pos	2744	261.2	2566-39-4;	151023	
g-Glutamylphenylalanine	1.15	1.01	1.11	Peptide	gamma-glutamyl	LC-MS Pos	2846	295.1	7432-24-8;	111299	
g-Glutamyltyrosine	1.19	1.02	0.93	Peptide	gamma-glutamyl	LC-MS Pos	2073	311.2	7432-23-7;	94340	
g-Glutamylvaline	0.98	1.02	1.25	Peptide	gamma-glutamyl	LC-MS Pos	2040	247.2	2746-34-1;		

Supplemental Data for:

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Supplemental Table 2 The complete exo-metabolome identified in this study. Compound names are reported, along with their CAS, PUBCHEM, and KEGG identifiers. The biological pathway to which the compound belongs, the method of identification, the retention index (RI), and the sizes of the metabolites are also listed. Normalized concentrations of each compound are shown for the three time points.

	Concentration								Identifier		
Compound	Day 4	Day 9	Day 15	Super pathway	Subpathway	Platform	RI	Mass	CAS	PUBCHEM	KEGG
Glycylleucine	0.52	1.51	1.66	Peptide	Dipeptide	LC-MS Pos	2236	189.1	869-19-2;	928,431,548,899	C02155
Isoleucylisoleucine	0.79	0.82	1.19	Peptide	Dipeptide	LC-MS Pos	2678	245.1	42537-99-5;		
Isoleucylleucine	0.93	1.91	6.87	Peptide	Dipeptide	LC-MS Pos	2856	245.1	26462-22-6;	11644431	
Leu-Leu-Leu	0.69	0.91	5.99	Peptide	Polypeptide	LC-MS Pos	3795	358.2	10329-75-6;	259327	
Leucylalanine	0.64	0.91	4.86	Peptide	Dipeptide	LC-MS Pos	1760	203.2	7298-84-2;	259321	
Leucylleucine	0.75	1.69	7.23	Peptide	Dipeptide	LC-MS Pos	3012	245.1	3303-31-9;	768,076,992,072	C11332
Phenylalanylleucine	0.41	0.88	4.21	Peptide	Dipeptide	LC-MS Pos	3273	279.2	3303-55-7;	4078229	
1,4-Butanediol	1.18	1.32	0.71	Xenobiotics	Chemical	GC-MS	1208	115.8	110-63-4;		
2-Pyrrolidinone	1.00	1.83	1.68	Xenobiotics	Chemical	GC-MS	1190.9	142	616-45-5;	12025	
3,4-Dihydroxybenzaldehyde	1.22	0.82	0.82	Xenobiotics	Food component/plant	GC-MS	1615	267.1	139-85-5;	8768	
3,4-Dihydroxyphenylethanol	0.53	1.18	1.43	Xenobiotics	Food component/plant	GC-MS	1727	267.1	10597-60-1;		
3-Deoxyoctulosonate	0.82	0.99	1.07	Xenobiotics	Bacterial	GC-MS	1942	373.2	103404-70-2;	4636210	
4-Hydroxy catechol	1.75	1.32	0.77	Xenobiotics	Benzoate metabolism	GC-MS	1599	342.2	533-73-3;	10787	C02814
Abscisate	1.01	0.94	0.92	Xenobiotics	Food component/plant	LC-MS Neg	3195	263.1	14375-45-2;	5280896	C06082
Allose	0.93	0.93	0.94	Xenobiotics	Food component/plant	GC-MS	1782.8	204	7283-09-2;	102288	C01487
Erythritol	0.64	1.23	1.30	Xenobiotics	Sugar, sugar substitute, starch	GC-MS	1517.5	217	149-32-6;		C00503
Galactarate (mucic acid)	0.92	1.02	1.01	Xenobiotics	Sugar, sugar substitute, starch	GC-MS	1899.3	333.1	526-99-8;	3037582	C00879
Galactonate	1.10	1.09	0.93	Xenobiotics	Food component/plant	LC-MS Neg	655	195.1	299-28-5;	128869	C00880
Galacturonate	0.63	1.02	1.20	Xenobiotics	Sugar, sugar substitute, starch	GC-MS	1888.7	204	91510-62-2;	84740	C08348
Glycolate (hydroxyacetate)	2.14	1.36	0.48	Xenobiotics	Chemical	GC-MS	1119	177	79-14-1;	3,698,251,757	C00160
Kaempferol 3-*O*-beta-glucoside	1.19	0.96	0.73	Xenobiotics	Food component/plant	LC-MS Pos	3884	449	480-10-4;		
Lidocaine	0.20	0.55	1.68	Xenobiotics	Drug	LC-MS Pos	2761	235.2	137-58-6;	3676	D00358
Luteolin-7-*O*-glucoside	1.38	1.02	0.87	Xenobiotics	Food component/plant	LC-MS Pos	3590	448.9	5373-11-5;	5280637	C03951
p-Aminobenzoate (PABA)	0.44	0.79	1.10	Xenobiotics	Benzoate metabolism	LC-MS Pos	2120	138.1	150-13-0;	7,057,990,978	C00568
Quercetin	1.06	1.12	1.59	Xenobiotics	Food component/plant	GC-MS	2318.5	647.4	849061-97-8;	5280343	C00389
Quercetin-3-galactoside	1.34	0.81	0.63	Xenobiotics	Food component/plant	LC-MS Neg	2706	463.2	482-36-0;	5281643	C10073
Quercetin-3-*O*-glucoside	1.21	0.90	0.92	Xenobiotics	Food component/plant	LC-MS Pos	3649	464.8	21637-25-2;		
Shikimate	0.88	0.88	1.04	Xenobiotics	Food component/plant	GC-MS	1758.1	204	138-59-0;	8742	C00493
Sophorose	0.61	1.08	0.99	Xenobiotics	Sugar, sugar substitute, starch	GC-MS	2193.1	204.1	20429-79-2;	88719	C08250
Tartarate	0.98	1.06	0.93	Xenobiotics	Food component/plant	GC-MS	1626.1	292.1	6106-24-7;	875	C00898
Trihydroxybutane	0.80	1.58	1.28	Xenobiotics	Food component/plant	GC-MS	1329.5	117	4435-50-1;	20497	