

Supporting information

A Novel Quantitative Metabolomic Approach for the Study of Stress Responses of Plant Root Metabolism

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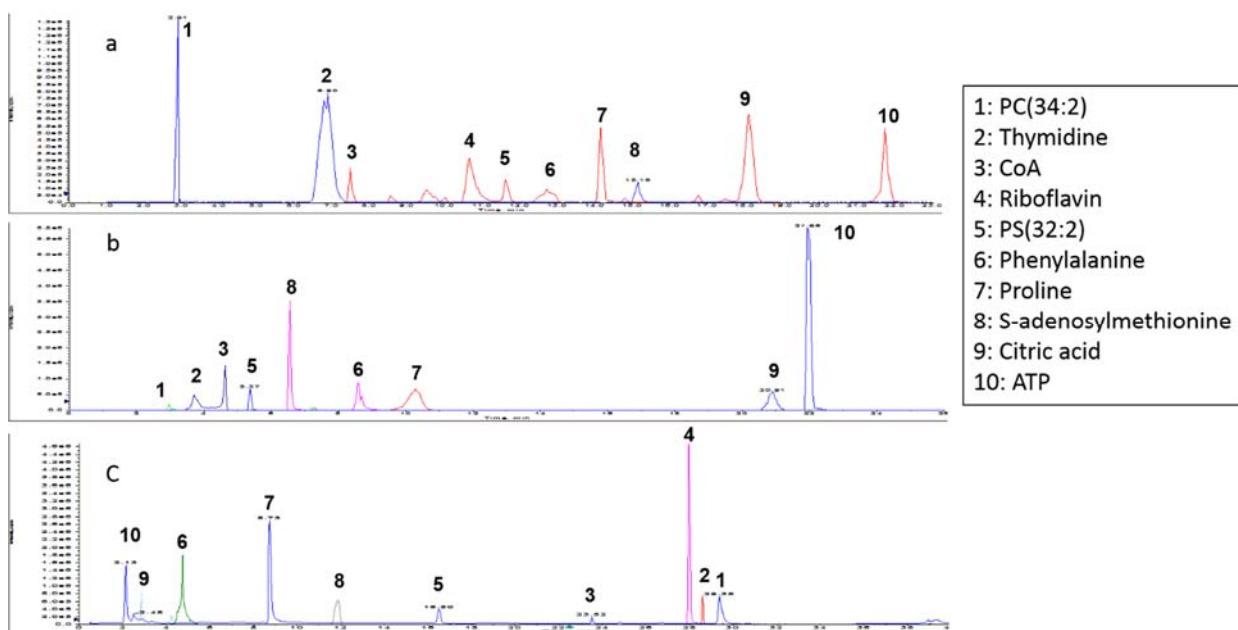


Figure S1 Extracted ion chromatograms of 10 representative compounds separated by three types of columns

(a): Acclaim Mixed-Mode HILIC-1 column (b):HILIC Luna NH₂ column (c):Synergi Fusion-RP column. Compound 7 was not detected on Luna NH₂ column.

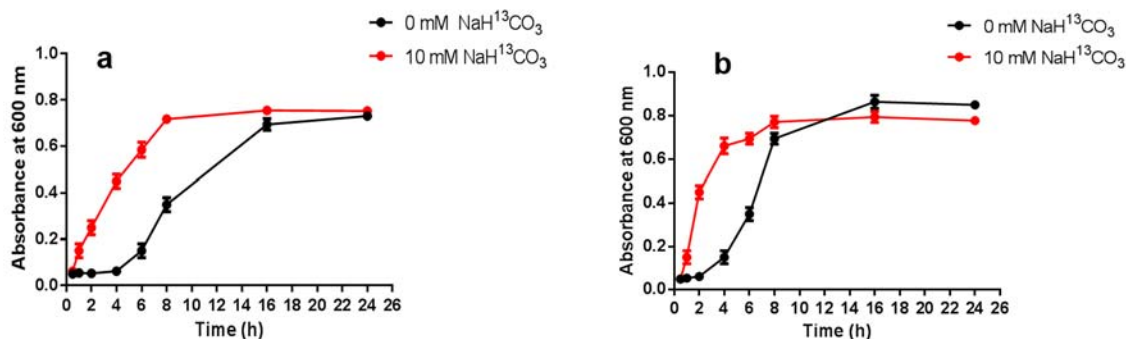


Figure S2 Effect of $\text{NaH}^{13}\text{CO}_3$ on *E. coli* (a) and yeast growth (b).

Metabolic active *E. coli* cells from a 3-ml culture were inoculated to 100 ml M9 medium supplemented with 0.1% of $[\text{U}-^{13}\text{C}]$ glucose as the carbon source. Absorbance at 600 nm was recorded at the time intervals (0.5, 1, 2, 4, 6, 8, 16 and 24 h). After 24 h, *E. coli* culture was centrifuged and the supernatant was sterilized by filtration. The supernatant was supplemented with 0.5% of uniformly $[\text{U}-^{13}\text{C}]$ glucose and 1x M9 salts for yeast growth. Metabolic active yeast cells from a 3-ml culture were then inoculated and cultured for another 24 h. The absorbance at 600 nm was recorded at the time intervals (0.5, 1, 2, 4, 6, 8, 16 and 24 h). Data points were mean $\pm$ SD of three batches of culture.

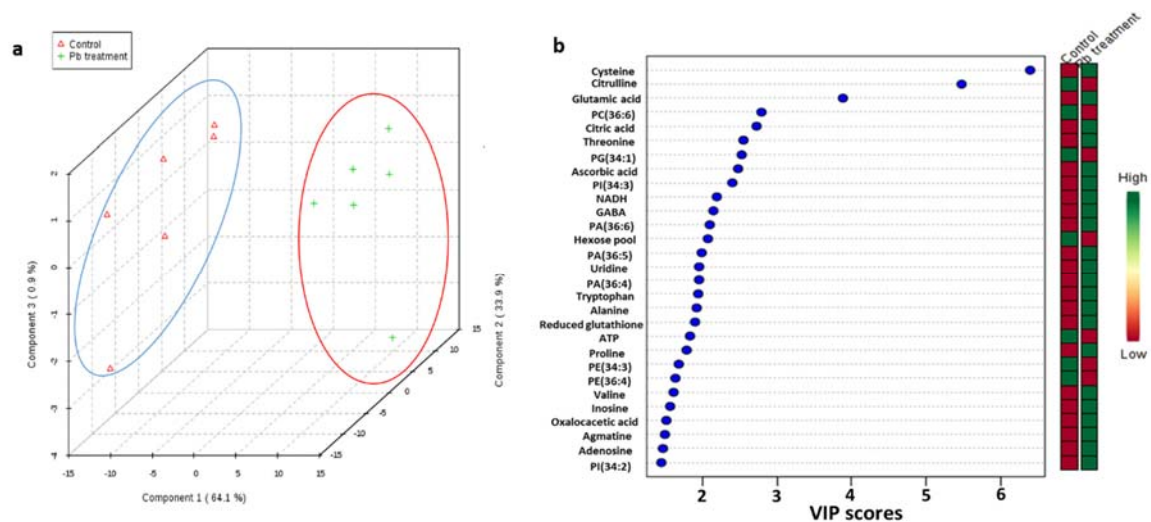


Figure S3 Changes of maize root metabolism in response to Pb treatment identified by targeted metabolomic analysis.

a: Partial least square analysis (PLS-DA) showed clear separation of maize root metabolism with and without Pb treatment. b: Top 30 metabolites changed by Pb treatment. Variable importance in projection (VIP) scores are a multivariate statistic that reflects the impact of each metabolite on PLS-DA model. VIP scores above 1.5 are significant.

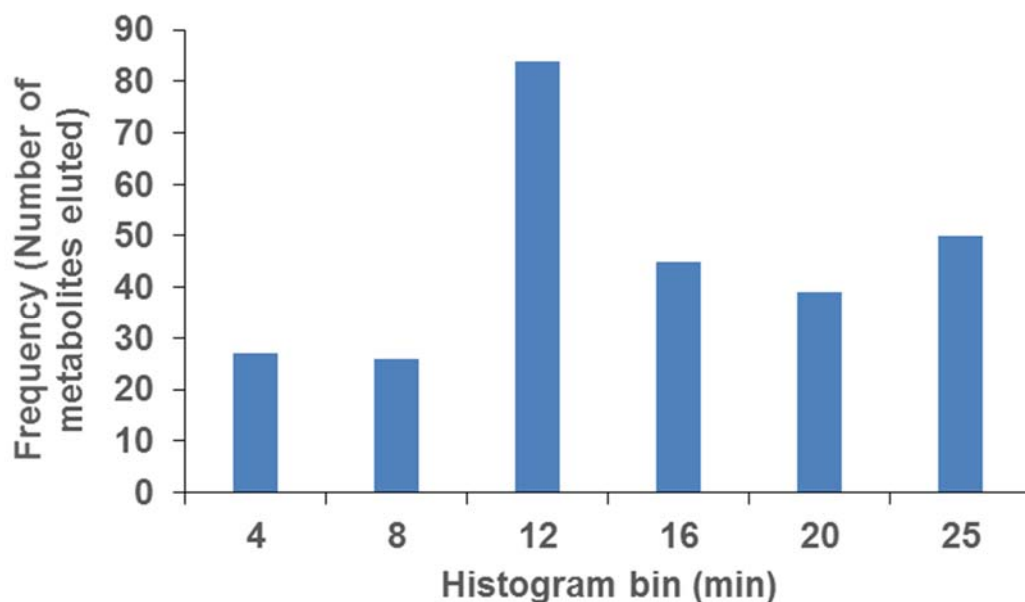


Figure S4 Histogram of metabolites elution order on Acclaim Mixed-Mode HILIC-1 column.

The chromatographic conditions were as follows: Mobile phase A was 95% H₂O with 20 mM ammonium formate and 5% acetonitrile (pH 4). Mobile phase B was 100% acetonitrile. The gradient was as follows: 0 min-95% B, 3 min-95% B, 3.1 min-85% B, 6.0 min-85% B, 6.1 min-75% B, 10 min-75% B, 15 min-0% B, 25 min-0%, 26 min-95% B, 31 min-end.

Table S1 List of targeted metabolites in this study

Component Name	Chemical classes	Unlabeled Formula	Q1 Labeled	Q3 Labeled	Q1_unlabeled	Q3_unlabeled	RT	DP	EP	CE	CXP
1-Pyrroline-5-carboxylic acid	Organic acids	C5H7NO2	119.2	70.7	114.2	67.7	12.3	56.3	7.94	19	11.2
2-Ketobutyric acid	Organic acids	C4H6O3	105	60.2	101	57.2	17.2	-93	-10	-13	-10
2-Keto-L-gluconate	Organic acids	C6H10O7	199	107	193	103	17.5	-90	-10	-12	-10
3-hydroxy-3-methylglutaryl-CoA	Cofactors	C27H44N7O20P3S	937	418	910	408	9.2	-90	-10	-63	-8
3-Phosphoglyceric acid	Organic phosphate	C3H7O7P	188	97	185	97	18.7	-90	-10	-15	-10
4,5 Dihydroorotic acid	Organic acids	C5H6N2O4	162	117	157	113	11.4	-90	-10	-12	-10
6-Phosphogluconic acid	Organic phosphate	C6H13O10P	281	79	275	97	14.59	-56.4	-10	-22	-5.24
Acetic acid	Organic acids	C2H4O2	61	61	59	59	10.5	-82.9	-9.8	-9.4	-27.23
Acetoacetic acid	Organic acids	C4H6O3	105	60	101	57	11.8	-38.4	-10	-14.7	-6.7
Acetoacetyl-CoA	Cofactors	C25H40N7O18P3S	877	360	852	345	10.1	93	10	36	10
Acetylcholine	Alcohols and Polyols	C7H15NO2	153.1	91	146.1	87	13.88	95	10	21	10
Acetyl-CoA	Cofactors	C23H38N7O17P3S	833	316	810	303	9.8	93	10	30	10
Acetylphosphate	Organic phosphate	C2H5O5P	141	63	139	63	18.2	-85	-10	-75.8	-7.2
Acrotic acid	Organic acids	C6H6O6	179.1	134	173.1	129	19.2	-20.5	-8.3	-11.5	-12
Adenine	Nucleosides, Nucleotides, and Analogues	C5H5N5	141.1	124	136.1	119	9.2	93	10	24	10
Adenosine	Nucleosides, Nucleotides, and Analogues	C10H13N5O4	278.2	141	268.2	136	8.52	93	10	27	10
Adenosine phosphosulfate	Nucleosides, Nucleotides, and Analogues	C10H14N5O10PS	436	356	426	346	21.5	-90	-10	-20	-10
ADP	Nucleosides, Nucleotides, and Analogues	C10H15N5O10P2	436.2	79	426.2	79	11	-100	-10	-80	-16
ADP-glucose	Nucleosides, Nucleotides, and Analogues	C16H25N5O15P2	604	356	588	346	21.7	-90	-10	-22	-10
Agmatine	Amino Acids and Derivatives	C5H14N4	136.2	76	131.2	72	11.4	60	10	21.2	12.24
Alanine	Amino Acids and Derivatives	C3H7NO2	93.1	46.2	90.1	44.2	12.9	93	10	13	10
Alpha-ketoisovaleric acid	Organic acids	C5H8O3	120	74	115	70	18.74	-93	-10	-13	-10
Aminoadipic acid	Amino Acids and Derivatives	C6H11NO4	166	148	160	142	17.9	-67.5	-10	-16	-11.8
AMP	Nucleosides, Nucleotides, and Analogues	C10H14N5O7P	358	141	348	136	21.5	50.34	10	27.16	20.8
Arginine	Amino Acids and Derivatives	C6H14N4O2	179.2	136	173.2	131	14.6	-125.3	-10	-19.1	-6.9
Ascorbic acid	Organic acids	C6H8O6	181.1	118.6	175.1	114.6	17.6	-66	-10	-20.8	-16
Asparagine	Amino Acids and Derivatives	C4H8N2O3	137.1	76	133.1	74	14.2	93	10	17	10
Aspartic acid	Amino Acids and Derivatives	C4H7NO4	136.1	91	132.1	88	17.5	-40.5	-10	-18.2	-9.2
ATP	Nucleosides, Nucleotides, and Analogues	C10H16N5O13P3	516.18	79	506.18	79	21.7	-69.09	-9.43	-131.55	-13.52
Benzoic acid	Organic acids	C7H6O2	129	83	121	77	21.5	-90	-10	-20	-10
Beta-alanine	Amino Acids and Derivatives	C3H7NO2	93.1	73.1	90.1	72.1	13.2	45.4	7.79	11.4	30.2
Carbamoyl-phosphate	Organic Phosphate	CH4NO5P	141	79	140	79	11.8	-90	-10	-22	-10
CDP	Nucleosides, Nucleotides, and Analogues	C9H15N3O11P2	411	79	402	79	21.5	-100	-10	-100	-23
Choline	Alcohols and Polyols	C5H14NO	109	63	104	60	13	93	10	19	10
Citric acid	Organic acids	C6H8O7	197	116	191	87	18.1	-90	-10	-13	-10
Citrulline	Amino Acids and Derivatives	C6H13N3O3	180	136	174	131	13.8	-76.4	-10	-19.1	-6.4
CMP	Nucleosides, Nucleotides, and Analogues	C9H14N3O8P	333	116	324	112	21.5	93	10	16	10
Coenzyme A	Cofactors	C21H36N7O16P3S	789	272	766	79.1	7.62	-180	-10	-134.1	-10.2
CTP	Nucleosides, Nucleotides, and Analogues	C9H16N3O14P3	491	79	482	79	21.7	-182	-10	-108	-17.4
cyclic AMP	Nucleosides, Nucleotides, and Analogues	C10H12N5O6P	338	139	328	134	15.5	-50	-7.2	-32.8	-9
Cystathionine	Amino Acids and Derivatives	C7H14N2O4S	230.26	138	223.26	134	16.8	93	10	11	10
Cysteine	Amino Acids and Derivatives	C3H7NO2S	125.26	61	122.26	59	11.2	93	10	27	10
Cytidine	Nucleosides, Nucleotides, and Analogues	C9H13N3O5	253	116	244	112	9.92	93	10	12	10
Cytosine	Nucleosides, Nucleotides, and Analogues	C4H5N3O	118	99	112.1	95	9	105	10	27.5	16.63
dADP	Nucleosides, Nucleotides, and Analogues	C10H15N5O9P2	420	79	410	79	21.3	-69.09	-9.43	-131.55	-13.52
dAMP	Nucleosides, Nucleotides, and Analogues	C10H14N5O6P	342	141	332	136	21.5	93	10	21	10
dATP	Nucleosides, Nucleotides, and Analogues	C10H16N5O12P3	500	79	490	79	21.7	-40.2	-10	-94	-9.2
dCDP	Nucleosides, Nucleotides, and Analogues	C9H15N3O10P2	395	79	386	79	11	-110	-10	-78.9	-9.2
dCMP	Nucleosides, Nucleotides, and Analogues	C9H14N3O7P	317	116	308	112	21.5	93	10	16	10
dCTP	Nucleosides, Nucleotides, and Analogues	C9H16N3O13P3	475	79	465.8	79	21.7	-182	-10	-108	-17.4
Deoxyadenosine	Nucleosides, Nucleotides, and Analogues	C10H13N5O3	262	141	252	136	7.54	93	10	20	10
Deoxyguanosine	Nucleosides, Nucleotides, and Analogues	C10H13N5O4	278.2	157.1	266.2	150.1	12.1	-86	-10	-28.1	-8
Deoxyinosine	Nucleosides, Nucleotides, and Analogues	C10H12N4O4	263	142	253	137	13.35	93	10	12	10
Deoxyribose phosphate	Sugar and Sugar Phosphate	C5H10O7P	218	79	121	79	21.3	-90	-10	-20	-10
Deoxyuridine	Nucleosides, Nucleotides, and Analogues	C9H12N2O5	238	117	229	113	9.16	93	10	11	10
Dephospho-CoA	Cofactors	C21H35N7O13P2S	709	358	688	348	9.9	93	10	25	10
dGDP	Nucleosides, Nucleotides, and Analogues	C10H15N5O10P2	436	79	426	79	21.6	-110	-10	-75.9	-13.4
dGMP	Nucleosides, Nucleotides, and Analogues	C10H14N5O7P	358	140	348	135	21.6	93	10	36	10
dGTP	Nucleosides, Nucleotides, and Analogues	C10H16N5O13P3	516.12	159	506.12	79	21.7	-110	-10	-110	-12
dIMP	Nucleosides, Nucleotides, and Analogues	C10H13N4O7P	341	79	331	79	21.4	-20	-10	-65	-9
dITP	Nucleosides, Nucleotides, and Analogues	C10H15N4O13P3	501	79	491.16	79	21.7	-24.1	-10	-104	-9.1
dTDP	Nucleosides, Nucleotides, and Analogues	C10H16N2O11P2	411	159	401	79	21.6	-93	-10	-100	-15.3
dTDP-D-Glucose	Nucleosides, Nucleotides, and Analogues	C16H26N2O16P2	579.3	331	563.3	321	21.6	-70	-10	-33.6	-23.1
dTMP	Nucleosides, Nucleotides, and Analogues	C10H15N2O8P	333	86	323	81	14.75	93	10	17	10
dTTP	Nucleosides, Nucleotides, and Analogues	C10H17N2O14P3	491.17	79	481.17	79	21.7	-93	-10	-100	-15.3
dUMP	Nucleosides, Nucleotides, and Analogues	C9H13N2O8P	316	200	307	195	21.7	-52.5	-10	-18	-12.9
dUTP	Nucleosides, Nucleotides, and Analogues	C9H15N2O14P3	476	159	467	159	21.7	-93	-10	-27	-9.9
Erythrose 4-phosphate	Sugar and Sugar Phosphate	C4H9O7P	203	97	199	97	21.5	-90	-10	-17	-10
Ethanolamine	Polyamines	C2H7NO	64.1	46	62.1	44	6.2	93	10	12	10
FAD	Nucleosides, Nucleotides, and Analogues	C27H33N9O15P2	813	358	786	348	19.5	93	10	26	10
Farnesyl diphosphate	Cofactors	C15H28O7P2	396.13	79	381.13	79	21.7	-97	-10	-77	-15
FMN	Cofactors	C17H21N4O9P	472	218	455	213	19.7	-90	-10	-19	-10
Fumaric acid	Organic acids	C4H4O4	119	74	115	71	17.9	-80.2	-10	-13	-10
Gamma-Aminobutyric acid	Amino Acids and Derivatives	C4H9NO2	144.1	73	104.1	69	14.7	93	10	22	10
GDP	Nucleosides, Nucleotides, and Analogues	C10H15N5O11P2	452	79	442	79	21.5	-110	-10	-75.9	-13.4
Geranyl-PP	Organic phosphate	C10H20O7P2	323	79	313	79	20.8	-90	-10	-20	-10
Glucuric acid	Organic acids	C6H10O8	215	88	209	85	19.5	-90	-10	-16	-4
Gluconic acid	Organic acids	C6H12O7	201	134	195	129	16.8	-90	-10	-15	-10
Glucosamine	Sugar and Sugar Phosphate	C6H13NO5	186	168	180	162	10.6	93	10	10	10
Glucosamine 6-phosphate	Sugar and Sugar Phosphate	C6H14NO8P	264	79	258	79	21.5	-54.3	-10	-63	-9.2
Glutaconic acid	Organic acids	C5H6O4	134.1	89	129.1	85	14.9	-37.9	-10	-11.3	-4.6
Glutamic acid	Amino Acids and Derivatives	C5H9NO4	153	88	148	84	18	93	10	15	10
Glutamine	Amino Acids and Derivatives	C5H10N2O3	152.1	88	147	84	13.5	93	10	15	10
Glyceraldehyde	Alcohols and Polyols	C3H6O3	91.8	61	88.8	59	10.5	-95	-10	-10	-10
Glyceraldehyde 3-phosphate	Organic phosphate	C3H7O6P	172	97	169	97	20.1	-36	-11	-15	-5.8

Glyceric acid	Organic acids	C3H6O4	108	77	105	75	16.4	-90	-10	-15	-10
Glycerol	Alcohols and Polyols	C3H8O3	96	59	93	57	18.6	95	10	12	10
Glycerol 3-phosphate	Organic Phosphate	C3H9O6P	174	79	171	79	21.2	-38.3	-10	-29.9	-9.4
Glycerophosphocholine	Alcohols and Polyols	C8H21NO6P	266.1	109	258.1	104	12.36	93	10	16	10
Glycine	Amino Acids and Derivatives	C2H5NO2	78.03	31.03	76.03	30.03	13.7	78	10	18	11.4
Glycolic acid	Organic acids	C2H4O3	77	46.2	75	45.2	16.2	-36.4	-10	-13.5	-9.16
Glyoxylic acid	Organic acids	C2H2O3	75	46	73	45	10.5	-93	-10	-22	-10
GMP	Nucleosides, Nucleotides, and Analogues	C10H14N5O8P	374	157	364	152	21.3	93	10	19	10
GTP	Nucleosides, Nucleotides, and Analogues	C10H16N5O14P3	532	79	522	79	21.7	-170	-10	-110	-12
Guanine	Nucleosides, Nucleotides, and Analogues	C5H5N5O	157	57	152	55	10.96	90	11	40.4	13
Guanosine	Nucleosides, Nucleotides, and Analogues	C10H13N5O5	291.9	155	281.9	150	12.1	-95	-10	-28.16	-10.14
Hexose bisphosphate	Sugar and Sugar Phosphate	C6H14O12P2	345	97	339	97	21.5	-93	-10	-30	-10
Hexose monophosphate	Sugar and Sugar Phosphate	C6H13O9P	265	79	259	79	20.1	-44	-10	-70	-9.2
Hexose pool	Sugar and Sugar Phosphate	C6H12O6	185	61	179	59	10.05	-36.2	-10	-23.1	-5.8
Histidine	Amino Acids and Derivatives	C6H9N3O2	162	115	156	110	14.64	93	10	12	10
Homocysteine	Amino Acids and Derivatives	C4H9NO2S	140	93	136	90	13.17	93	10	10	10
Homoserine	Amino Acids and Derivatives	C4H9NO3	124	46	120	44	14.2	90	10	32	10
Hydroxyphenyllactic acid	Organic acids	C9H10O4	190	143	181	135	14.5	-41.5	-10	-23.9	-7
Hypoxanthine	Nucleosides, Nucleotides, and Analogues	C5H4N4O	142	114	135	92	12.3	-93	-10	-18	-10
IDP	Nucleosides, Nucleotides, and Analogues	C10H14N4O11P2	437	159	427	79	21.6	-46	-10	-106	-9.1
IMP	Nucleosides, Nucleotides, and Analogues	C10H13N4O8P	359	142	349	137	21.4	93	10	19	10
Inosine	Nucleosides, Nucleotides, and Analogues	C10H12N4O5	279	142	267	135	12.6	-93	-10	-27	-10
Isoleucine	Amino Acids and Derivatives	C6H13NO2	138.2	91	132.2	86	10.7	93	10	11	10
ITP	Nucleosides, Nucleotides, and Analogues	C10H15N4O14P3	517	79	507	79	9.8	-46	-10	-106	-9.1
Lactic acid	Organic acids	C3H6O3	92.1	45.2	89.1	43.2	14.1	-93	-10	-16	-10
Leucine	Amino Acids and Derivatives	C6H13NO2	138.2	91	132.2	86	10.7	93	10	11	10
Lysine	Amino Acids and Derivatives	C6H14N2O2	153.1	89.1	147.1	84.1	13.8	93	10	15	10
LysoPC(16:0)	Phospholipids	C24H50NO7P	520	189	496	184	7.8	35	10	45	27
LysoPC(18:0)	Phospholipids	C26H54NO7P	550	189	524	184	7.7	35	10	45	27
LysoPC(22:0)	Phospholipids	C30H62NO7P	624.4	189	594.4	184	3.5	40	10	47	9
Malic acid	Organic acids	C4H6O5	137	119	133	115	18.5	-55	-4	-15	-5.4
Malonyl-CoA	Cofactors	C24H38N7O19P3S	878	361	854	347	11.2	93	10	28	10
Methionine	Amino Acids and Derivatives	C5H11NO2S	155	63	150	61	11.3	93	10	30	10
Myoinositol	Sugar and Sugar Phosphate	C6H12O6	185	47	179.16	161	11.5	-93	-10	-17	-11.2
N-Acetyl-glucosamine 1-phosphate	Sugar and Sugar Phosphate	C8H16NO9P	308	79	300	79	21.2	-90	-10	-32	-10
N-Acetylornithine	Amino Acids and Derivatives	C7H14N2O3	182.2	120	175.2	115	13.5	93	10	14	10
N-acetylserine	Amino Acids and Derivatives	C5H9NO4	151.1	120	146.05	116	15.9	-46.1	-10	-14.1	-6.06
NAD+	Nucleosides, Nucleotides, and Analogues	C21H28N7O14P2	683	555	662	540	17.7	-42.1	-10	-26.7	-11.9
NADH	Nucleosides, Nucleotides, and Analogues	C21H29N7O14P2	685	79	664	408	21.4	-93	-10	-33	-12.7
NADP+	Nucleosides, Nucleotides, and Analogues	C21H29N7O17P3	763	635	742	620	21.2	-32.5	-10	-25.8	-11
NADPH	Nucleosides, Nucleotides, and Analogues	C21H30N7O17P3	765	79	744	79	21.2	-93	-10	-36	-10
Niacinamide	Vitamins and Derivatives	C6H6N2O	129	85	123	80	4.4	93	10	20	10
Nicotinic acid	Vitamins and Derivatives	C6H5NO2	128	83	122	78	17.6	-90	-10	-14	-10
Oleic acid	Fatty acids	C18H34O2	299.2	74	281.2	71	9.2	-128	-10	-68	-28
Ornithine	Amino Acids and Derivatives	C5H12N2O2	138	74	133	70	15.7	93	10	12	10
Orotidylic acid	Nucleosides, Nucleotides, and Analogues	C10H13N2O11P	377	332	319	97	21.5	-90	-10	-22	-10
Oxalic acid	Organic acids	C2H2O4	90.6	61.5	88.6	60.5	17.8	-20.6	-10	-11.9	-6.82
Oxaloacetic acid	Organic acids	C4H4O5	135	90	131	87	18.4	-47	-9	-12.8	-13
Oxidized glutathione	Amino Acids and Derivatives	C20H32N6O12S2	633	239	613	231	19.1	93	10	35	10
Oxoglutaric acid	Organic acids	C5H6O5	150.1	105	145.1	101	18.2	-93	-12	-13.8	-5.93
PA(28:0)	Phospholipids	C31H61O8P	622.4	181.1	591.4	171.1	9.8	-80	-10	-50	-13
PA(28:1)	Phospholipids	C31H59O8P	620.4	211.2	589.4	199.2	9.8	-80	-10	-50	-13
PA(30:0)	Phospholipids	C33H65O8P	652.4	211.2	619.4	199.2	9.8	-80	-10	-50	-13
PA(30:1)	Phospholipids	C33H63O8P	650.4	241.2	617.4	227.2	9.8	-80	-10	-50	-13
PA(32:0)	Phospholipids	C35H69O8P	682.4	271.2	647.4	255.2	9.8	-80	-10	-50	-13
PA(32:1)	Phospholipids	C35H67O8P	680.4	241.2	645.4	227.2	9.8	-80	-10	-50	-13
PA(32:2)	Phospholipids	C35H65O8P	678.4	269.2	643.4	253.2	9.8	-80	-10	-50	-13
PA(34:1)	Phospholipids	C37H71O8P	710.5	269.2	673.5	253.2	9.8	-80	-10	-50	-13
PA(34:2)	Phospholipids	C37H69O8P	708.5	299.3	671.5	281.3	9.8	-180	-10	-50	-13
PA(34:3)	Phospholipids	C37H67O8P	706.5	299.3	669.5	281.3	9.8	-180	-10	-50	-13
PA(36:1)	Phospholipids	C39H75O8P	740.5	299.3	701.5	281.3	9.71	-180	-10	-50	-13
PA(36:2)	Phospholipids	C39H73O8P	738.5	299.3	699.5	281.3	9.71	-80	-10	-50	-13
PA(36:4)	Phospholipids	C39H69O8P	734.5	299.3	695.5	281.3	9.71	-80	-10	-50	-13
PA(36:5)	Phospholipids	C39H67O8P	732.5	299.3	693.5	281.3	9.71	-80	-10	-50	-13
PA(36:6)	Phospholipids	C39H65O8P	730.5	299.3	691.5	281.3	9.71	-80	-10	-50	-13
p-Aminobenzoic acid	Organic acids	C7H7NO2	143	98	136	92	16.9	-90	-10	-16	-10
Pantothenic acid	Vitamins and Derivatives	C9H17NO5	227	152	218	146	14.5	-90	-10	-19	-10
PC(22:0)	Phospholipids	C30H60NO8P	624.4	189.1	594.4	184.1	3.5	40	10	47	9
PC(22:1)	Phospholipids	C30H58NO8P	622.4	189.1	592.4	184.1	3.5	40	10	47	9
PC(24:0)	Phospholipids	C32H64NO8P	654.4	189.1	622.4	184.1	3.5	40	10	47	
PC(24:1)	Phospholipids	C32H62NO8P	652.4	189.1	620.4	184.1	3.6	40	10	47	
PC(26:0)	Phospholipids	C34H68NO8P	684.6	189.1	650.5	184.1	3.3	40	10	47	9
PC(26:1)	Phospholipids	C34H66NO8P	682.6	189.1	648.5	184.1	3.5	40	10	47	9
PC(28:0)	Phospholipids	C36H72NO8P	714.5	189.1	678.5	184.1	3.5	40	10	47	9
PC(28:1)	Phospholipids	C36H70NO8P	712.5	189.1	676.5	184.1	3.3	40	10	47	9
PC(28:2)	Phospholipids	C36H68NO8P	710.5	189.1	674.5	184.1	3.3	40	10	47	9
PC(30:0)	Phospholipids	C38H76NO8P	744.5	189.1	706.5	184.1	3.1	40	10	47	9
PC(30:1)	Phospholipids	C38H74NO8P	742.5	189.1	704.5	184.1	3.1	40	10	47	9
PC(30:2)	Phospholipids	C38H72NO8P	740.5	189.1	702.5	184.1	3.1	40	10	47	9
PC(32:0)	Phospholipids	C40H80NO8P	774.6	189.1	734.6	184.1	3.1	40	10	47	9
PC(32:1)	Phospholipids	C40H78NO8P	772.6	189.1	732.6	184.1	3.1	40	10	47	9
PC(32:2)	Phospholipids	C40H76NO8P	770.5	189.1	730.5	184.1	3.1	40	10	47	9
PC(34:1)	Phospholipids	C42H82NO8P	802.6	189.1	760.6	184.1	3.1	40	10	47	11
PC(34:2)	Phospholipids	C42H80NO8P	800.6	189.1	758.6	184.1	3.1	40	10	47	11
PC(34:3)	Phospholipids	C42H78NO8P	798.6	189.1	756.6	184.1	3.1	40	10	47	11
PC(36:0)	Phospholipids	C44H88NO8P	834.6	189.1	790.6	184.1	3.1	40	10	47	9
PC(36:1)	Phospholipids	C44H86NO8P	832.6	189.1	788.6	184.1	3.2	40	10	47	9
PC(36:2)	Phospholipids	C44H84NO8P	830.6	189.1	786.6	184.1	3.1	40	10	47	13

PC(36:3)	Phospholipids	C44H82NO8P	828.6	189.1	784.6	184.1	3.1	40	10	47	13
PC(36:4)	Phospholipids	C44H80NO8P	826.5	189.1	782.5	184.1	3.1	40	10	47	13
PC(36:5)	Phospholipids	C44H78NO8P	824.5	189.1	780.5	184.1	3.1	40	10	47	13
PC(36:6)	Phospholipids	C44H76NO8P	822.5	189.1	778.5	184.1	3.1	40	10	47	13
PC(38:3)	Phospholipids	C46H86NO8P	858.6	189.1	812.6	184.1	3.1	40	10	47	13
PC(38:5)	Phospholipids	C46H82NO8P	854.6	189.1	808.6	184.1	3.1	35	10	45	27
PE(28:0)	Phospholipids	C33H66NO8P	667.4	211.2	634.4	199.2	7.6	-50	-10	-48	-11
PE(28:1)	Phospholipids	C33H64NO8P	667.4	211.2	632.4	199.2	7.6	-45	-10	-48	-11
PE(30:0)	Phospholipids	C35H70NO8P	697.5	241.2	662.5	227.2	7.4	-50	-10	-48	-11
PE(30:1)	Phospholipids	C35H68NO8P	695.5	211.2	660.5	199.2	7.4	-45	-10	-48	-11
PE(30:2)	Phospholipids	C35H66NO8P	693.5	239.2	658.5	225.2	7.4	-50	-10	-48	-11
PE(32:1)	Phospholipids	C37H72NO8P	725.5	241.2	688.5	227.2	7.8	-45	-10	-48	-11
PE(32:2)	Phospholipids	C37H70NO8P	723.5	269.2	686.5	253.2	7.4	-45	-10	-48	-11
PE(34:1)	Phospholipids	C39H76NO8P	755.5	271.2	716.5	255.2	7.3	-45	-10	-48	-11
PE(34:2)	Phospholipids	C39H74NO8P	753.5	299.3	714.5	281.3	7.2	-45	-10	-50	-15
PE(34:3)	Phospholipids	C39H72NO8P	751.5	299.3	712.5	281.3	7.4	-45	-10	-50	-15
PE(36:1)	Phospholipids	C41H80NO8P	785.5	299.3	744.5	281.3	7.3	-45	-10	-50	-15
PE(36:2)	Phospholipids	C41H78NO8P	783.5	299.3	742.5	281.3	7.3	-45	-10	-48	-11
PE(36:3)	Phospholipids	C41H76NO8P	781.5	299.3	740.5	281.3	7.3	-45	-10	-50	-15
PE(36:4)	Phospholipids	C41H74NO8P	779.5	299.3	738.5	281.3	7.3	-45	-10	-50	-15
PG(32:0)	Phospholipids	C38H75O10P	759.5	269.2	721.5	253.2	9.67				
PG(32:1)	Phospholipids	C38H73O10P	757.5	269.2	719.5	253.2	9.67	-160	-10	-48	-17
PG(32:2)	Phospholipids	C38H71O10P	755.5	269.2	717.5	253.2	9.67	-160	-10	-48	-17
PG(34:1)	Phospholipids	C40H77O10P	787.5	269.2	747.5	255.2	9.95	-160	-10	-48	-17
PG(34:2)	Phospholipids	C40H75O10P	785.5	269.2	745.5	253.2	9.97	-160	-10	-48	-17
Phenylalanine	Amino Acids and Derivatives	C9H11NO2	175	128	166.1	120.08	11	93	10	28	10
Phenyllactic acid	Organic acids	C9H10O3	174	156	165	147	10.5	-93	-10	-16.8	-10
Phenylpyruvic acid	Organic acids	C9H8O3	172	98	163	91	10.5	-93	-10	-21	-11
Phosphoenolpyruvic acid	Organic Phosphate	C3H5O6P	170	79	167	79	18.9	-90	-10	-25.1	-9.2
Phosphoribosyl pyrophosphate	Organic phosphate	C5H13O14P3	394	177	389	177	21.6	-21.6	-10	-25.72	-15.91
Phosphorylcholine	Alcohols and Polyols	C5H15NO4P	189	128	184	125	19	93	10	23	10
Phosphoserine	Organic phosphate	C3H8NO6P	189	91	186	88	15.2	93	10	12	10
PI(26:0)	Phospholipids	C35H67O13P	760.5	181.1	725.5	171.1	11.8	-40	-10	-62	-10
PI(28:0)	Phospholipids	C37H71O13P	790.6	211.2	753.6	199.2	11.8	-40	-10	-62	-10
PI(28:1)	Phospholipids	C37H69O13P	788.6	239.2	751.6	225.2	11.8	-40	-10	-62	-10
PI(30:0)	Phospholipids	C39H75O13P	820.6	211.2	781.6	199.2	11.8	-40	-10	-62	-10
PI(30:1)	Phospholipids	C39H73O13P	818.6	239.2	779.6	225.2	11.8	-40	-10	-62	-10
PI(30:2)	Phospholipids	C39H71O13P	816.6	269.2	777.6	253.2	11.8	-50	-10	-62	-10
PI(32:0)	Phospholipids	C41H79O13P	841.6	271.2s	809.6	255.2	11.5	-50	-10	-62	-10
PI(32:1)	Phospholipids	C41H77O13P	848.6	239.2	807.6	225.2	11.8	-40	-10	-62	-10
PI(32:2)	Phospholipids	C41H75O13P	846.6	269.2	805.6	253.2	11.8	-50	-10	-62	-10
PI(34:0)	Phospholipids	C43H83O13P	880.7	271.2	837.7	255.2	11.8	-50	-10	-62	-10
PI(34:1)	Phospholipids	C43H81O13P	878.6	299.3	835.6	281.3	11.5	-50	-10	-62	-10
PI(34:2)	Phospholipids	C43H79O13P	876.6	299.3	833.6	253.2	11.5	-50	-10	-62	-10
PI(34:3)	Phospholipids	C43H77O13P	874.6	299.3	831.6	253.2	11.5	-50	-10	-62	-10
PI(36:1)	Phospholipids	C45H85O13P	908.7	299.3	863.7	281.3	11.8	-50	-10	-62	-10
PI(36:2)	Phospholipids	C45H83O13P	906.7	299.3	861.7	281.3	11.5	-50	-10	-62	-10
Prephenate	Organic acids	C10H10O6	235	97	225	91	18	-50	-10	-15	-10
Proline	Amino Acids and Derivatives	C5H9NO2	121	74	116	70	12	93	10	11	10
Propionyl-CoA	Cofactors	C24H40N7O17P3S	848	331	824	317	8.5	93	10	35	10
PS(32:0)	Phospholipids	C38H74NO10P	766.5	271.2	734.5	255.2	11.2	-115	-10	-60	-5
PS(32:1)	Phospholipids	C38H72NO10P	764.5	271.2	732.5	253.2	11.2	-90	-10	-60	-33
PS(32:2)	Phospholipids	C38H70NO10P	768.5	269.2	730.5	253.2	11.2	-90	-10	-60	-33
PS(34:1)	Phospholipids	C40H76NO10P	800.6	271.2	760.6	255.2	11.2	-90	-10	-60	-33
PS(34:2)	Phospholipids	C40H74NO10P	798.6	269.2	758.6	253.2	11.2	-90	-10	-60	-33
PS(34:3)	Phospholipids	C40H72NO10P	796.6	269.2	756.6	253.2	11.2	-90	-10	-60	-33
PS(36:0)	Phospholipids	C42H82NO10P	832.5	301.3	790.5	283.3	11.2	-115	-10	-60	-33
PS(36:2)	Phospholipids	C42H78NO10P	828.5	299.3	786.5	283.3	11.2	-115	-10	-60	-33
Putrescine	Polyamines	C4H12N2	93.1	76	89.1	72	16.2	40	10	12.7	15
Pyridoxine	Vitamins and Derivatives	C8H11NO3	178	142	170	134	10.1	93	10	22	10
Pyroglutamic acid	Amino Acids and Derivatives	C5H7NO3	133	86	128	82.1	15.15	-61.3	-10	-16.8	-10.2
Pyruvic acid	Organic acids	C3H4O3	90	45	87	43	14.5	-46	-8	-14	-15
Quinolinic acid	Organic acids	C7H5NO4	173	128	166	122	18.2	-90	-10	-12	-10
Reduced glutathione	Amino Acids and Derivatives	C10H17N3O6S	318	167	306	143	18.8	-93	-10	-19	-10
Riboflavin	Vitamins and Derivatives	C17H20N4O6	394	255	377	243	10.9	90	10	24	10
Ribose 5-phosphate	Sugar and Sugar Phosphate	C5H11O8P	234	97	229	97	21.5	-41.3	-12	-17	-6
S-Adenosylhomocysteine	Amino Acids and Derivatives	C14H20N6O5S	399	141	385	136	14.8	93	10	19	
S-Adenosylmethionine	Amino Acids and Derivatives	C15H23N6O5S	414.1	259	399.1	250	13.8	95	11.21	23.04	10.16
Sarcosine	Amino Acids and Derivatives	C3H7NO2	93.09	46	90.09	44	12.88	93	10	19.11	17.26
Sedoheptulose monophosphate	Sugar and Sugar Phosphate	C7H15O10P	296	97	289	97	21.2	-93	-10	-27	-10
Serine	Amino Acids and Derivatives	C3H7NO3	109	62	106	60	14.57	93	10	13	10
Shikimic acid	Organic acids	C7H10O5	180.2	99	173.2	93	10.49	-90	-10	-18	-10
Spermidine	Polyamines	C7H19N3	153.1	119	146.1	112	17.1	62	10	20.34	20.05
Succinic acid	Organic acids	C4H6O4	121	103	117.09	99	18.9	-42	-10	-14	-10
Succinyl-CoA	Cofactors	C25H40N7O19P3S	893	376.1	868	361.1	13.6	93	10	40	10
Sucrose	Sugar and Sugar Phosphate	C12H22O11	353.3	185	341.3	179	11.3	-93	-10	-20	-10
Thiamine	Vitamins and Derivatives	C12H17N4OS	277	128	265	122	9.18	93	10	17	10
Thiamine monophosphate	Vitamins and Derivatives	C12H17N4O4PS	357	128	345	122	18.8	93	10	13	10
Threonine	Amino Acids and Derivatives	C4H9NO3	122	77	118	74	13.1	-46.5	-10	-14.2	-6.7
Thymidine	Nucleosides, Nucleotides, and Analogues	C10H14N2O5	251	130	241	125	6.9	-90	-10	-15	-10
Thymine	Nucleosides, Nucleotides, and Analogues	C5H6N2O2	132	115	127	110	6.6	93	10	17	10
Tryptophan	Amino Acids and Derivatives	C11H12N2O2	216	155	205	146	11.2	70	10	21	12
Tyramine	Polyamines	C8H11NO	145.9	83	137.9	77	7.8	44.83	6.95	34.6	20.54
Tyrosine	Amino Acids and Derivatives	C9H11NO3	191	144	182	136	12.9	93	10	37	10
UDP	Nucleosides, Nucleotides, and Analogues	C9H14N2O12P2	412	314	402.7	79	21.5	-100	-10	-82	-23
UDP-D-glucose	Nucleosides, Nucleotides, and Analogues	C15H24N2O17P2	580	332	565	323	21.6	-90	-10	-23	-10
UDP-n-acetyl-D-glucosamine	Nucleosides, Nucleotides, and Analogues	C17H27N3O17P2	623	394	606	385	21.7	-90	-10	-26	-10
UMP	Nucleosides, Nucleotides, and Analogues	C9H13N2O9P	332	79	323	79	21.5	-95	-8	-89	-23

Uracil	Nucleosides, Nucleotides, and Analogues	C4H4N2O2	115	43.1	111	42.1	6.8	-93	-10	-22	-10
Ureidosuccinic acid	Amino Acids and Derivatives	C5H8N2O5	180	135	175	132	14	-90	-10	-12	-10
Uridine	Nucleosides, Nucleotides, and Analogues	C9H12N2O6	252	43.1	242.91	42.1	9.16	-110	-10	-52	-7
Uridine diphosphate glucuronic acid	Nucleosides, Nucleotides, and Analogues	C15H22N2O18P2	594	412	579	403	21.5	-90	-10	-24	-10
UTP	Nucleosides, Nucleotides, and Analogues	C9H15N2O15P3	492	79	483	79	21.7	-130	-10	-134.6	-12.18
Valine	Amino Acids and Derivatives	C5H11NO2	123	76	118.15	72	11.2	60	10	17	11.99
Xanthine	Nucleosides, Nucleotides, and Analogues	C5H4N4O2	158.1	114	151.11	108	16	-93	-10	-23	-10
Xanthosine	Nucleosides, Nucleotides, and Analogues	C10H12N4O6	295	158	282.7	151	17.9	-55	-10	-33.89	-18.44
Xanthylic acid	Nucleosides, Nucleotides, and Analogues	C10H13N4O9P	375	102	365	97	17.5	93	10	11	10

Table S2 The absolute concentration of uniformly ¹³C labeled metabolites in *E.coli*-yeast culture

Metabolites	Chemical classes	Standard curves	Coefficient r	Concentration in <i>E.coli</i> -yeast culture (ng/mg dry weight)
1-Pyrroline-5-carboxylic acid-13C	Organic acids	y=0.11915x+0.04077	0.9818	49.46±3.82
2-Ketobutyric acid-13C	Organic acids	y=0.006705x+0.02787	0.9801	19.50±2.91
2-Keto-L-gluconate-13C	Organic acids	y=0.1914x+0.02419	0.9800	8.31±4.82
3-hydroxy-3-methylglutaryl-CoA-13C	Cofactors	y=0.008581x+0.0004061	0.9886	140.14±3.28
3-Phosphoglyceric acid-13C	Organic phosphate	y=0.1091x+0.2843	0.9948	444.41±32.95
4,5-Dihydroorotic acid-13C	Organic acids	y=0.08788x+0.005682	0.9821	48.67±4.11
6-Phosphogluconic acid-13C	Organic phosphate	y=0.3373x+0.1911	0.9960	4919.15±870.55
Acetic acid-13C	Organic acids	y=1.321x+0.4358	0.9925	30414.51±3215.93
Acetoacetic acid-13C	Organic acids	y=0.2276x-0.003906	0.9820	59.61±6.82
Acetoacetyl-CoA-13C	Cofactors	y=0.02979x+0.008664	0.9883	224.92±18.79
Acetylcholine-13C	Alcohols and Polyols	y=0.8299x-0.013517	0.9946	0.22±0.041
Acetyl-CoA-13C	Cofactors	y=0.1003x+0.003014	0.9884	898.71±75.98
Acetylphosphate-13C	Organic phosphate	y=0.8299x-1.3517	0.9956	2461.13±194.57
Aconitic acid-13C	Organic acids	y=0.01074x+0.0001309	0.9965	1438.46±299.15
Adenine-13C	Nucleosides, Nucleotides, and Analogues	y=0.4919x+0.02243	0.9973	1055.83±31.78
Adenosine phosphosulfate-13C	Nucleosides, Nucleotides, and Analogues	y=0.027816x+0.008224	0.9960	61.77±4.31
Adenosine-13C	Nucleosides, Nucleotides, and Analogues	y=1.2186x+0.06437	0.9977	6989.65±742.53
ADP-13C	Nucleosides, Nucleotides, and Analogues	y=1.9415x+0.04689	0.9969	4185.28±396.74
ADP-glucose-13C	Nucleosides, Nucleotides, and Analogues	y=0.02983x+0.006044	0.9859	48.22±1.05
Agmatine-13C	Amino Acids and Derivatives	y=0.03197x+0.0173	0.9925	23.61±0.79
Alanine-13C	Amino Acids and Derivatives	y=1.4576x-2.6284	0.9920	14711.53±781.68
Alpha-ketoisovaleric acid-13C	Organic acids	y=0.003062x+0.1783	0.9994	39.1±1.98
Aminoadipic acid-13C	Amino Acids and Derivatives	y=0.007927x+0.02475	0.9892	2.88±0.51
AMP-13C	Nucleosides, Nucleotides, and Analogues	y=1.15305x+0.1283	0.9947	19716.16±1582.91
Arginine-13C	Amino Acids and Derivatives	y=1.2371x+0.1351	0.9998	12305.86±1053.77
Ascorbic acid-13C	Organic acids	y=0.04547x+0.004403	0.9986	214.67±19.58
Asparagine-13C	Amino Acids and Derivatives	y=3.251x-0.1236	0.9905	1891.16±159.13
Aspartic acid-13C	Amino Acids and Derivatives	y=1.2856x-0.0676	0.9993	10096.96±389.73
ATP-13C	Nucleosides, Nucleotides, and Analogues	y=0.1824x+1.456	0.9979	37704.52±3108.69
Benzoic acid-13C	Organic acids	y=1.225x+0.01564	0.9985	27.36±5.31
Beta-alanine-13C	Amino Acids and Derivatives	y=0.06682x+0.0018254	0.9917	52.26±5.97
Carbamoyl-phosphate-13C	Organic Phosphate	y=0.0273x+0.4153	0.9963	1330.84±325.96
CDP-13C	Nucleosides, Nucleotides, and Analogues	y=0.09642x+0.001028	0.9939	1157.76±302.39
Choline-13C	Alcohols and Polyols	y=2.671x+0.000013	0.9949	1026.08±132.38
Citric acid-13C	Organic acids	y=15.91x+0.0005028	0.9992	58000.67±1421.56
Citrulline-13C	Amino Acids and Derivatives	y=0.8699x+0.08649	0.9911	6264.01±143.9
CMP-13C	Nucleosides, Nucleotides, and Analogues	y=0.5249x+0.04093	0.9958	2553.12±151.67
Coenzyme A-13C	Cofactors	y=0.0363x+0.0285	0.9889	930.42±58.39
CTP-13C	Nucleosides, Nucleotides, and Analogues	y=0.1355x+0.01681	0.9938	5701.63±1326.34
cyclic AMP-13C	Nucleosides, Nucleotides, and Analogues	y=0.1298x+0.00166	0.9964	472.32±36.51
Cystathionine-13C	Amino Acids and Derivatives	y=0.01106x+0.002461	0.9893	5.13±0.61
Cysteine-13C	Amino Acids and Derivatives	y=0.779x-0.01128	0.9930	431.57±38.42
Cytidine-13C	Nucleosides, Nucleotides, and Analogues	y=0.1958x+0.014141	0.9972	15.25±0.91
Cytosine-13C	Nucleosides, Nucleotides, and Analogues	y=0.2437x+0.02316	0.9977	29.71±3.26
dADP-13C	Nucleosides, Nucleotides, and Analogues	y=0.0396x+0.00006992	0.9877	325.95±15.63
dAMP-13C	Nucleosides, Nucleotides, and Analogues	y=0.06229x+0.0022915	0.9858	263.94±22.31
dATP-13C	Nucleosides, Nucleotides, and Analogues	y=0.3964x-0.05313	0.9933	467.46±32.85
dCDP-13C	Nucleosides, Nucleotides, and Analogues	y=3.4710x+0.001974	0.9969	148.22±11.14
dCMP-13C	Nucleosides, Nucleotides, and Analogues	y=0.56388x+0.02259	0.9858	182.95±13.51
dCTP-13C	Nucleosides, Nucleotides, and Analogues	y=0.01264x+0.0002379	0.9947	244.08±21.54
Deoxyadenosine-13C	Nucleosides, Nucleotides, and Analogues	y=0.06214x-0.000462	0.9879	31.25±3.58
Deoxyguanosine-13C	Nucleosides, Nucleotides, and Analogues	y=0.001337x+0.000011131	0.9969	19.69±2.72
Deoxyinosine-13C	Nucleosides, Nucleotides, and Analogues	y=0.011161x+0.000006928	0.9966	13.62±0.31
Deoxyribose phosphate-13C	Sugar and Sugar Phosphate	y=0.04743x+0.005992	0.9981	733.51±28.98
Deoxyuridine-13C	Nucleosides, Nucleotides, and Analogues	y=0.4986x-0.0002788	0.9977	13.28±0.65
Dephospho-CoA-13C	Cofactors	y=0.0011x-0.01236	0.9884	447.26±36.41
dGDP-13C	Nucleosides, Nucleotides, and Analogues	y=0.1281x+0.01103	0.9946	24.71±1.08
dGMP-13C	Nucleosides, Nucleotides, and Analogues	y=0.001405x+0.001244	0.9946	271.44±13.56
dGTP-13C	Nucleosides, Nucleotides, and Analogues	y=0.2215x+0.039158	0.9931	141.71±19.28
dIMP-13C	Nucleosides, Nucleotides, and Analogues	y=0.24152x+0.003952	0.9935	6.95±0.17
dITP-13C	Nucleosides, Nucleotides, and Analogues	y=0.1543x-0.3808	0.9945	5.41±0.52
dTDP-13C	Nucleosides, Nucleotides, and Analogues	y=0.19609x+0.007916	0.9953	2197.48±321.69
dUDP-D-Glucose-13C	Nucleosides, Nucleotides, and Analogues	y=0.03643x+2.435	0.9852	55.26±4.39
dTMP-13C	Nucleosides, Nucleotides, and Analogues	y=0.1824x+0.02131	0.9965	69.93±1.72
dTTP-13C	Nucleosides, Nucleotides, and Analogues	y=0.1243x+0.03466	0.9937	9531.97±325.64
dUMP-13C	Nucleosides, Nucleotides, and Analogues	y=0.07424x+0.0009294	0.9945	65.08±7.93
dUTP-13C	Nucleosides, Nucleotides, and Analogues	y=0.02386x+0.01722	0.9944	13.94±1.38
Erythrose 4-phosphate-13C	Sugar and Sugar Phosphate	y=0.002178x+0.05006	0.9914	12.14±2.73

Ethanolamine-13C	Polyamines	$y=0.01384x+0.0009406$	0.9926	19.37±3.38
FAD-13C	Nucleosides, Nucleotides, and Analogues	$y=0.14427x+0.0040854$	0.9937	1204.15±79.59
Farnesyl diphosphate-13C	Cofactors	$y=0.5014x+0.09443$	0.9882	247.74±36.81
FMN-13C	Cofactors	$y=0.04681x+0.005011$	0.9982	488.67±75.32
Fumaric acid-13C	Organic acids	$y=0.5856x+0.01668$	0.9985	557.17±79.01
Gamma-Aminobutyric acid-13C	Amino Acids and Derivatives	$y=0.009372x+0.004264$	0.9895	86.41±7.63
GDP-13C	Nucleosides, Nucleotides, and Analogues	$y=0.2184x-0.07534$	0.9936	3771.14±325.69
Geranyl-PP-13C	Organic phosphate	$y=0.1258x+0.018293$	0.9939	1476.11±325.63
Glucaric acid-13C	Organic acids	$y=0.16177x+0.005384$	0.9963	80.67±15.88
Gluconic acid-13C	Organic acids	$y=0.1618x+0.0005384$	0.9906	184.27±31.33
Glucosamine 6-phosphate-13C	Sugar and Sugar Phosphate	$y=0.00771x+0.0002029$	0.9812	5341.89±369.52
Glucosamine-13C	Sugar and Sugar Phosphate	$y=0.22x+0.04310$	0.9836	68.72±5.88
Glutaconic acid-13C	Organic acids	$y=0.02816x+0.00984$	0.9913	18.97±7.82
Glutamic acid-13C	Amino Acids and Derivatives	$y=0.4986x-0.05347$	0.9991	11905.76±3241.55
Glutamine-13C	Amino Acids and Derivatives	$y=1.622x+0.0025903$	0.9911	31075.81±535.39
Glyceraldehyde 3-phosphate-13C	Organic phosphate	$y=0.7085x+0.003266$	0.9948	320.63±65.85
Glyceraldehyde-13C	Alcohols and Polyols	$y=0.4223x+0.0002$	0.9951	44.41±3.12
Glyceric acid-13C	Organic acids	$y=0.3263x+0.0002038$	0.9911	2961.71±273.63
Glycerol 3-phosphate-13C	Organic Phosphate	$y=0.7995x+0.01122$	0.9953	841.63±15.77
Glycerol-13C	Alcohols and Polyols	$y=0.9193x+0.027$	0.9941	2369.64±109.7
Glycerophosphocholine-13C	Alcohols and Polyols	$y=0.2562x+0.0007$	0.9950	61.84±1.25
Glycine-13C	Amino Acids and Derivatives	$y=0.1077x+0.0376$	0.9911	1223.31±78.54
Glycolic acid-13C	Organic acids	$y=1.1258x+0.02747$	0.9913	211.51±38.26
Glyoxylic acid-13C	Organic acids	$y=0.8103x+0.01615$	0.9925	101.84±37.41
GMP-13C	Nucleosides, Nucleotides, and Analogues	$y=0.2415x+0.01674$	0.9935	193.65±21.77
GTP-13C	Nucleosides, Nucleotides, and Analogues	$y=0.2373x+0.003156$	0.9930	37260.61±488.31
Guanine-13C	Nucleosides, Nucleotides, and Analogues	$y=0.1883x+0.00004256$	0.9971	452.96±31.23
Guanosine-13C	Nucleosides, Nucleotides, and Analogues	$y=0.01731x-0.008915$	0.9968	191.69±11.32
Hexose bisphosphate-13C	Sugar and Sugar Phosphate	$y=1.165x+0.3801$	0.9997	12954.88±1708.53
Hexose monophosphate-13C	Sugar and Sugar Phosphate	$y=4.897x+0.1308$	0.9998	7071.99±412.69
Hexose pool-13C	Sugar and Sugar Phosphate	$y=9.936x+0.006423$	0.9996	11396.57±2190.78
Histidine-13C	Amino Acids and Derivatives	$y=0.1722x+0.03391$	0.9997	8132.28±361.57
Homocysteine-13C	Amino Acids and Derivatives	$y=0.1645x+0.01356$	0.9918	708.56±63.29
Homoserine-13C	Amino Acids and Derivatives	$y=0.01679x+0.007204$	0.9900	45.62±3.15
Hydroxyphenyllactic acid-13C	Organic acids	$y=0.01763x+0.02162$	0.9814	115.16±21.44
Hypoxanthine-13C	Nucleosides, Nucleotides, and Analogues	$y=0.4283x-0.0003355$	0.9967	734.44±32.91
IDP-13C	Nucleosides, Nucleotides, and Analogues	$y=0.1543x-0.3808$	0.9950	798.51±56.28
IMP-13C	Nucleosides, Nucleotides, and Analogues	$y=0.09851x-0.01637$	0.9934	2041.65±139.82
Inosine-13C	Nucleosides, Nucleotides, and Analogues	$y=0.4371x-0.00012982$	0.9967	154.86±27.43
Isoleucine-13C	Amino Acids and Derivatives	$y=10.0409x+0.001933$	0.9934	2782.81±457.63
ITP-13C	Nucleosides, Nucleotides, and Analogues	$y=0.1543x-0.3808$	0.9972	2585.7±217.13
Lactic acid-13C	Organic acids	$y=2.913x+0.0008827$	0.9915	3624.59±152.82
Leucine-13C	Amino Acids and Derivatives	$y=0.9814x-0.02699$	0.9932	2514.44±309.15
Lysine-13C	Amino Acids and Derivatives	$y=0.311x-0.0231$	0.9907	5695.71±531.56
LysoPC(16:0)-13C	Phospholipids	$y=16.28192x+0.02058$	0.9961	22.61±9.15
LysoPC(18:0)-13C	Phospholipids	$y=12.0233x+0.006324$	0.9970	22.74±7.32
LysoPC(22:0)-13C	Phospholipids	$y=0.04398x+0.007898$	0.9926	8.49±1.54
Malic acid-13C	Organic acids	$y=0.001268x+0.0005162$	0.9988	7773.85±298.79
Malonyl-CoA-13C	Cofactors	$y=0.001395x+0.0003158$	0.9883	558.52±15.79
Methionine-13C	Amino Acids and Derivatives	$y=1.2153x+0.03251$	0.9926	1012.51±109.53
Myoinositol-13C	Sugar and Sugar Phosphate	$y=0.1005x+0.0001091$	0.9917	20.61±4.28
N-Acetyl-glucosamine 1-phosphate-13C	Sugar and Sugar Phosphate	$y=0.001781x+0.01991$	0.9809	492.91±33.64
N-Acetylmethionine-13C	Amino Acids and Derivatives	$y=0.0383x+0.001343$	0.9911	481.82±35.67
N-acetylsarcosine-13C	Amino Acids and Derivatives	$y=0.06971x+0.007435$	0.9894	51.11±4.68
NAD ⁺ -13C	Nucleosides, Nucleotides, and Analogues	$y=0.08393x+0.001167$	0.9962	8967.22±538.75
NADH-13C	Nucleosides, Nucleotides, and Analogues	$y=0.1169x+0.003571$	0.9999	7357.21±262.56
NADP ⁺ -13C	Nucleosides, Nucleotides, and Analogues	$y=0.1352x+0.03067$	0.9957	1461.74±105.32
NADPH-13C	Nucleosides, Nucleotides, and Analogues	$y=0.13523x+0.03067$	0.9944	1644.24±191.38
Niacinamide-13C	Vitamins and Derivatives	$y=0.6596x+0.005206$	0.9896	151.29±38.87
Nicotinic acid-13C	Vitamins and Derivatives	$y=0.1941x+0.01126$	0.9973	3834.46±517.62
Oleic acid-13C	Phospholipids	$y=0.0202x+0.0004324$	0.9738	0.28±0.11
Ornithine-13C	Amino Acids and Derivatives	$y=0.5791x+0.09028$	0.9995	9360.54±319.25
Orotidylic acid-13C	Nucleosides, Nucleotides, and Analogues	$y=0.001503x+0.2393$	0.9842	12.12±1.85
Oxalic acid-13C	Organic acids	$y=1.8201x+0.01839$	0.9975	112.91±38.53
Oxaloacetic acid-13C	Organic acids	$y=0.03668x+0.0002431$	0.9794	72.61±5.38
Oxidized glutathione-13C	Amino Acids and Derivatives	$y=0.4711x+0.001121$	0.9990	5464.22±403.61
Oxoglutaric acid-13C	Organic acids	$y=1.563x+0.03231$	0.9871	4516.96±291.34
PA(28:0)-13C	Phospholipids	$y=0.57217x+0.001685$	0.9923	5.32±1.05
PA(28:1)-13C	Phospholipids	$y=0.005363x+0.0009035$	0.9911	6.48±0.93
PA(30:0)-13C	Phospholipids	$y=0.08016x+0.0006569$	0.9910	2.47±0.51
PA(30:1)-13C	Phospholipids	$y=0.03305x+0.003361$	0.9809	1.23±0.48

PA(32:0)-13C	Phospholipids	$y=0.02299x+0.002698$	0.9803	1.94±0.22
PA(32:1)-13C	Phospholipids	$y=0.01478x+0.006405$	0.9802	8.39±1.01
PA(32:2)-13C	Phospholipids	$y=0.03417x+0.0008315$	0.9997	61.12±3.77
PA(34:1)-13C	Phospholipids	$y=0.02299+0.0002698$	0.9696	34.30±4.15
PA(34:2)-13C	Phospholipids	$y=0.05916x+0.009505$	0.9876	65.81±7.56
PA(34:3)-13C	Phospholipids	NA	NA	NA
PA(36:1)-13C	Phospholipids	$y=0.3526x+0.0009372$	0.9931	12.63±3.01
PA(36:2)-13C	Phospholipids	$y=0.03582x+0.0001369$	0.9894	3.49±0.72
PA(36:4)-13C	Phospholipids	NA	NA	NA
PA(36:5)-13C	Phospholipids	NA	NA	NA
PA(36:6)-13C	Phospholipids	NA	NA	NA
p-Aminobenzoic acid-13C	Organic acids	$y=0.13576x+0.002926$	0.9806	15.36±2.98
Pantothenic acid-13C	Vitamins and Derivatives	$y=0.1371x-0.03129$	0.9900	12.55±3.02
PC(22:0)-13C	Phospholipids	$y=1.0575x+0.004334$	0.9923	27.34±11.15
PC(22:1)-13C	Phospholipids	$y=1.6768x+0.11833$	0.9921	24.28±3.82
PC(24:0)-13C	Phospholipids	$y=8.3101x+0.02593$	0.9920	51.65±8.19
PC(24:1)-13C	Phospholipids	$y=1.4451x+0.18065$	0.9918	44.66±5.92
PC(26:0)-13C	Phospholipids	$y=1.7659x+0.01802$	0.9996	14.31±2.16
PC(26:1)-13C	Phospholipids	$y=0.2860x+0.002759$	0.9913	16.21±3.88
PC(28:0)-13C	Phospholipids	$y=0.26592x+0.05634$	0.9908	16.96±3.40
PC(28:1)-13C	Phospholipids	$y=4.036x+0.007079$	0.9900	16.35±20.66
PC(28:2)-13C	Phospholipids	$y=0.50749x+0.00058$	0.9992	14.83±5.52
PC(30:0)-13C	Phospholipids	$y=0.7407x+0.005667$	0.9986	12.72±3.84
PC(30:1)-13C	Phospholipids	$y=6.831x+0.04773$	0.9701	90.11±6.91
PC(30:2)-13C	Phospholipids	$y=4.3713x+0.008472$	0.9984	57.60±12.35
PC(32:0)-13C	Phospholipids	$y=2.5523x+0.00885$	0.9984	38.14±4.55
PC(32:1)-13C	Phospholipids	$y=1.5551x+2.7113$	0.9981	5381.48±535.33
PC(32:2)-13C	Phospholipids	$y=2.552x+0.00885$	0.9978	5926.54±377.14
PC(34:1)-13C	Phospholipids	$y=14.8682x+0.07632$	0.9676	314.13±28.86
PC(34:2)-13C	Phospholipids	$y=13.4215x+0.08069$	0.9837	6093.83±291.55
PC(34:3)-13C	Phospholipids	NA	NA	NA
PC(36:0)-13C	Phospholipids	$y=3.8873x+0.0132$	0.9708	10.27±1.93
PC(36:1)-13C	Phospholipids	$y=9.53576x+0.04513$	0.9972	11.83±2.54
PC(36:2)-13C	Phospholipids	$y=9.5357x+0.04513$	0.9830	14.15±5.09
PC(36:3)-13C	Phospholipids	NA	NA	NA
PC(36:4)-13C	Phospholipids	$y=1.4868x+0.07632$	0.9974	6.26±3.11
PC(36:5)-13C	Phospholipids	NA	NA	NA
PC(36:6)-13C	Phospholipids	NA	NA	NA
PC(38:3)-13C	Phospholipids	$y=2.72251x+0.008163$	0.9726	6.50±1.92
PC(38:5)-13C	Phospholipids	$y=2.7225x+0.008163$	0.9708	6.46±2.73
PE(28:0)-13C	Phospholipids	$y=1.5558x+0.2711$	0.9755	643.43±98.72
PE(28:1)-13C	Phospholipids	$y=0.3693x+0.7644$	0.9952	835.99±80.58
PE(30:0)-13C	Phospholipids	$y=1.555x+0.027113$	0.9949	474.35±96.48
PE(30:1)-13C	Phospholipids	$y=0.5669x+0.07676$	0.9847	208.718±35.63
PE(30:2)-13C	Phospholipids	$y=0.2426x+0.04757$	0.9948	139.61±17.54
PE(32:1)-13C	Phospholipids	$y=0.5712x-0.001230$	0.9846	7049.63±329.61
PE(32:2)-13C	Phospholipids	$y=0.01233x+0.0002135$	0.9948	21130.932±756.54
PE(34:1)-13C	Phospholipids	$y=0.05669x+0.007676$	0.9845	223.55±18.78
PE(34:2)-13C	Phospholipids	$y=0.03693x+0.0007$	0.9661	9361.38±850.05
PE(34:3)-13C	Phospholipids	NA	NA	NA
PE(36:1)-13C	Phospholipids	$y=0.5712x-0.01231$	0.9957	224.84±35.63
PE(36:2)-13C	Phospholipids	$y=0.05712x-0.001230$	0.9839	172.26±18.27
PE(36:3)-13C	Phospholipids	NA	NA	NA
PE(36:4)-13C	Phospholipids	NA	NA	NA
PG(32:0)-13C	Phospholipids	NA	NA	NA
PG(32:1)-13C	Phospholipids	$y=0.06508x+0.04281$	0.9937	8.63±1.49
PG(32:2)-13C	Phospholipids	$y=0.02442x+0.003561$	0.9932	8.61±2.25
PG(34:1)-13C	Phospholipids	$y=0.04484x+0.0001202$	0.9948	285.54±34.91
PG(34:2)-13C	Phospholipids	$y=0.012804x+0.002306$	0.9847	269.87±31.32
Phenylalanine-13C	Amino Acids and Derivatives	$y=17.93x+0.02122$	0.9932	2468.24±137.71
Phenyllactic acid-13C	Organic acids	$y=0.05875x+0.05597$	0.9823	30.19±2.56
Phenylpyruvic acid-13C	Organic acids	$y=0.0589x+0.3377$	0.9822	461.29±18.73
Phosphoenolpyruvic acid-13C	Organic Phosphate	$y=0.658x+0.001023$	0.9944	386.31±42.62
Phosphoribosyl pyrophosphate-13C	Organic phosphate	$y=0.5684x-0.08531$	0.9945	121.83±20.49
Phosphorylcholine-13C	Alcohols and Polyols	$y=0.5219x+0.000007$	0.9939	23.92±0.58
Phosphoserine-13C	Organic phosphate	$y=2.576x+0.001351$	0.9960	40.11±2.33
PI(26:0)-13C	Phospholipids	$y=0.05488x+0.0009988$	0.9944	23.21±4.88
PI(28:0)-13C	Phospholipids	$y=2.6564x-0.004241$	0.9842	9.04±1.75
PI(28:1)-13C	Phospholipids	$y=0.0514x+0.001197$	0.9925	9.01±0.99
PI(30:0)-13C	Phospholipids	$y=0.2804x+0.0002701$	0.9923	25.01±3.82
PI(30:1)-13C	Phospholipids	$y=0.4135x+0.1568$	0.9920	24.94±4.11

PI(30:2)-13C	Phospholipids	$y=0.03147x+0.001296$	0.9919	24.88±5.62
PI(32:0)-13C	Phospholipids	$y=0.0223x+0.001527$	0.9976	28.33±7.24
PI(32:1)-13C	Phospholipids	$y=0.1571x+0.03128$	0.9911	189.78±31.66
PI(32:2)-13C	Phospholipids	$y=0.04871x+0.001609$	0.9492	92.64±19.54
PI(34:0)-13C	Phospholipids	$y=0.02144x+0.01197$	0.9985	37.69±3.62
PI(34:1)-13C	Phospholipids	$y=0.2804x+0.00027$	0.9970	121.16±35.48
PI(34:2)-13C	Phospholipids	$y=0.02144x+0.001197$	0.9655	62.52±13.24
PI(34:3)-13C	Phospholipids	NA	NA	NA
PI(36:1)-13C	Phospholipids	$y=0.01168x+0.0004091$	0.9980	64.77±23.06
PI(36:2)-13C	Phospholipids	$y=0.01021x+0.00003301$	0.9954	12.92±1.58
Prephenate-13C	Organic acids	$y=0.01172x+0.1357$	0.9799	18.67±3.11
Proline-13C	Amino Acids and Derivatives	$y=0.3250x+0.1680$	0.9922	1644.88±325.74
Propionyl-CoA-13C	Cofactors	$y=0.09152x+0.007086$	0.9888	126.89±8.25
PS(32:0)-13C	Phospholipids	$y=0.003956x+0.002881$	0.9872	1.46±0.38
PS(32:1)-13C	Phospholipids	$y=0.04781x+0.003291$	0.9671	10.98±1.77
PS(32:2)-13C	Phospholipids	$y=0.05305x+0.004257$	0.9665	20.45±3.71
PS(34:1)-13C	Phospholipids	$y=0.0662x+0.0001517$	0.9948	13.69±4.05
PS(34:2)-13C	Phospholipids	$y=0.07136x+0.0002398$	0.9847	14.41±2.29
PS(34:3)-13C	Phospholipids	NA	NA	NA
PS(36:0)-13C	Phospholipids	$y=0.001393x+0.0002272$	0.9740	2.37±0.15
PS(36:2)-13C	Phospholipids	$y=0.006138x+0.0002986$	0.9934	1.57±0.85
Putrescine-13C	Polyamines	$y=0.1845x+0.0002848$	0.9901	1869.49±310.25
Pyridoxine-13C	Vitamins and Derivatives	$y=0.011653x+0.001856$	0.9922	9.79±1.05
Pyroglutamic acid-13C	Amino Acids and Derivatives	$y=0.01398x-0.002955$	0.9895	5.35±0.18
Pyruvic acid-13C	Organic acids	$y=2.072x+0.031$	0.9914	11571.59±2083.22
Quinolinic acid-13C	Organic acids	$y=0.5335x+0.005942$	0.9965	27.68±3.19
Reduced glutathione-13C	Amino Acids and Derivatives	$y=0.3421x+0.001038$	0.9991	7261.65±208.38
Riboflavin-13C	Vitamins and Derivatives	$y=0.08462x+0.0001534$	0.9901	93.34±7.15
Ribose 5-phosphate-13C	Sugar and Sugar Phosphate	$y=0.1719x+0.07857$	0.9970	57.93±10.03
S-Adenosylhomocysteine-13C	Amino Acids and Derivatives	$y=0.4296x+0.03393$	0.9995	435.58±43.24
S-Adenosylmethionine-13C	Amino Acids and Derivatives	$y=1.735x+0.01368$	0.9906	937.88±78.21
Sarcosine-13C	Amino Acids and Derivatives	$y=1.539x-0.00024$	0.9920	45.84±3.29
Sedoheptulose monophosphate-13C	Sugar and Sugar Phosphate	$y=0.005701x+0.0001022$	0.9880	44.22±3.09
Serine-13C	Amino Acids and Derivatives	$y=0.1832x-3.279$	0.9999	2068.06±171.31
Shikimic acid-13C	Organic acids	$y=5.404x+0.003765$	0.9925	46.21±10.11
Spermidine-13C	Polyamines	$y=0.8305x+0.002175$	0.9997	5930.49±715.61
Succinic acid-13C	Organic acids	$y=1.9768x+0.04728$	0.9982	13123.96±1415.79
Succinyl-CoA-13C	Cofactors	$y=0.01068x+0.003823$	0.9883	3033.26±56.91
Sucrose-13C	Sugar and Sugar Phosphate	$y=0.03063x+0.0002063$	0.9995	18.08±2.94
Thiamine monophosphate-13C	Vitamins and Derivatives	$y=0.2361x+0.006176$	0.9988	5.09±1.11
Thiamine-13C	Vitamins and Derivatives	$y=0.9425x+0.03937$	0.9937	3.91±0.46
Threonine-13C	Amino Acids and Derivatives	$y=0.3018x-8.278$	0.9919	1709.82±321.76
Thymidine-13C	Nucleosides, Nucleotides, and Analogues	$y=0.014x+0.00000712$	0.9980	16.38±2.93
Thymine-13C	Nucleosides, Nucleotides, and Analogues	$y=0.201x+0.000027$	0.9982	3.56±0.91
Tryptophan-13C	Amino Acids and Derivatives	$y=0.6175x+0.006685$	0.9930	557.61±32.79
Tyramine-13C	Polyamines	$y=0.1391x+0.02876$	0.9909	12.68±1.54
Tyrosine-13C	Amino Acids and Derivatives	$y=0.0013x+0.0000029$	0.9920	1734.46±256.89
UDP-13C	Nucleosides, Nucleotides, and Analogues	$y=0.01679x+0.007204$	0.9934	2530.605±81.93
UDP-D-glucose-13C	Nucleosides, Nucleotides, and Analogues	$y=0.2503x-0.008295$	0.9857	5147.65±435.32
UDP-n-acetyl-D-glucosamine-13C	Nucleosides, Nucleotides, and Analogues	$y=0.1883x+0.00004256$	0.9856	3994.42±392.35
UMP-13C	Nucleosides, Nucleotides, and Analogues	$y=0.7886x+0.01429$	0.9955	655.69±54.28
Uracil-13C	Nucleosides, Nucleotides, and Analogues	$y=0.1051x+0.0001018$	0.9981	2023.97±318.53
Ureidosuccinic acid-13C	Amino Acids and Derivatives	$y=0.03015x+0.006332$	0.9906	313.57±32.65
Uridine diphosphate glucuronic acid-13C	Nucleosides, Nucleotides, and Analogues	$y=0.05135x+0.008737$	0.9839	5896.53±378.42
Uridine-13C	Nucleosides, Nucleotides, and Analogues	$y=0.4504x-0.0004251$	0.9975	7027.38±521.65
UTP-13C	Nucleosides, Nucleotides, and Analogues	$y=2.6053x-0.0093252$	0.9948	5013.32±483.97
Valine-13C	Amino Acids and Derivatives	$y=9.8124x+0.0006$	0.9929	19014.84±432.15
Xanthine-13C	Nucleosides, Nucleotides, and Analogues	$y=0.1757x+0.003759$	0.9963	17.89±3.71
Xanthosine-13C	Nucleosides, Nucleotides, and Analogues	$y=0.31658x+0.07428$	0.9961	34.81±7.84
Xanthylic acid-13C	Nucleosides, Nucleotides, and Analogues	$y=0.1438x+0.0002855$	0.9963	12.08±2.95

Table S3 The stability of uniformly ¹³C labeled metabolites

Metabolites	Chemical classes	AUC_0 d	AUC_7 d	AUC_1 month	AUC_6 month	AUC_1 year	RSD(%)	Log2_AUC_0d	Log2_AUC_7d	Log_AUC_1 month	Log_AUC_6 month	Log_AUC_1 year	RSD of Log_AUC (%)
1-Pyrroline-5-carboxylic acid-13C	Organic acids	7.29E+04	7.20E+04	7.38E+04	7.44E+04	7.16E+04	1.61%	16.15402694	16.13610998	16.17172412	16.18340277	16.1280749	0.14%
2-Ketobutyric acid-13C	Organic acids	4.54E+05	4.14E+05	4.64E+05	4.04E+05	4.39E+05	5.87%	18.79360331	18.65961968	18.82376528	18.62542347	18.74517534	0.45%
2-Keto-L-gluconate-13C	Organic acids	5.28E+04	5.08E+04	5.19E+04	5.35E+04	5.31E+04	2.06%	15.68743036	15.63225685	15.66455839	15.70752091	15.69696753	0.19%
3-Phosphoglyceric acid-13C	Organic phosphate	1.93E+06	1.98E+06	1.85E+06	1.91E+06	1.85E+06	2.75%	20.87717627	20.91415152	20.82220981	20.86211669	20.81987346	0.19%
4,5-Dihydroxotric acid-13C	Organic acids	4.90E+04	4.52E+04	4.70E+04	4.92E+04	4.80E+04	3.46%	15.57961058	15.5307729	15.51975909	15.5866639	15.55074679	0.32%
6-Phosphogluconic acid-13C	Organic phosphate	5.46E+05	5.32E+05	5.41E+05	5.39E+05	5.40E+05	0.93%	19.05774852	19.02025294	19.04468883	19.03939033	19.04286702	0.07%
Acetic acid-13C	Organic acids	1.33E+07	1.31E+07	1.32E+07	1.38E+07	1.37E+07	2.33%	23.65948902	23.63754647	23.64855962	23.71292828	23.70239762	0.14%
Acetoacetic acid-13C	Organic acids	4.28E+05	4.42E+05	4.31E+05	4.20E+05	4.32E+05	1.81%	18.70859895	18.75401321	18.71866665	18.68140314	18.72100571	0.14%
Acetoacetyl-CoA-13C	Cofactors	3.56E+05	3.43E+05	3.06E+05	3.15E+05	3.36E+05	6.18%	18.44111241	18.38742838	18.22270058	18.26453423	18.35767227	0.49%
Acetylcholine-13C	Alcohols and Polyols	7.55E+05	7.45E+05	7.23E+05	7.59E+05	7.48E+05	1.88%	19.52649924	19.50726815	19.46403515	19.53431048	19.51306444	0.14%
Acetyl-CoA-13C	Cofactors	3.68E+05	3.79E+05	3.42E+05	3.39E+05	3.18E+05	6.97%	18.4901301	18.53259944	18.38448023	18.37177664	18.2957431	0.55%
Acetylphosphate-13C	Organic phosphate	3.23E+05	3.21E+05	3.18E+05	3.28E+05	3.32E+05	1.72%	18.30072792	18.29266314	18.27821349	18.32333629	18.3403891	0.14%
Acronitic acid-13C	Organic acids	6.92E+07	6.98E+07	6.81E+07	6.63E+07	6.74E+07	2.05%	26.04447717	26.05693038	26.0213633	25.98272312	26.00645929	0.11%
Adenine-13C	Nucleosides, Nucleotides, and Analogues	6.72E+05	6.77E+05	6.65E+05	6.58E+05	6.79E+05	1.31%	19.35831638	19.36943547	19.34321175	19.3279473	19.37368933	0.10%
Adenosine phosphosulfate-13C	Nucleosides, Nucleotides, and Analogues	8.13E+05	8.21E+05	7.73E+05	8.39E+05	8.21E+05	3.01%	19.63073227	19.64719841	19.56029551	19.67848323	19.64719841	0.22%
Adenosine-13C	Nucleosides, Nucleotides, and Analogues	1.34E+07	1.40E+07	1.43E+07	1.40E+07	1.31E+07	3.52%	23.67033641	23.73376179	23.76445858	23.73376179	23.64085921	0.22%
ADP-13C	Nucleosides, Nucleotides, and Analogues	1.60E+07	1.51E+07	1.48E+07	1.52E+07	1.66E+07	4.67%	23.92922228	23.84555896	23.82240434	23.85509811	23.98241849	0.28%
ADP-glucose-13C	Nucleosides, Nucleotides, and Analogues	5.16E+05	5.19E+05	5.08E+05	5.11E+05	5.23E+05	1.18%	18.97673192	18.98565296	18.95418495	18.96268141	18.99617554	0.09%
Agmatine-13C	Amino Acids and Derivatives	6.46E+05	6.53E+05	6.41E+05	6.41E+05	6.36E+05	1.00%	19.30162123	19.31716527	19.28973974	19.2904149	19.27912085	0.07%
Alanine-13C	Amino Acids and Derivatives	3.43E+06	3.19E+06	3.38E+06	3.23E+06	3.40E+06	3.22%	21.71061812	21.66029222	21.68944523	21.62399577	21.69498014	0.22%
Alpha-ketoglutaric acid-13C	Organic acids	8.04E+05	7.89E+05	8.54E+05	8.15E+05	8.24E+05	2.98%	19.61737419	19.59021422	19.70438326	19.63626351	19.65280997	0.22%
Aminoadipic acid-13C	Amino Acids and Derivatives	2.91E+05	2.83E+05	2.61E+05	2.96E+05	2.73E+05	5.02%	18.15016377	18.10993265	17.99313742	18.17572496	18.05906979	0.40%
AMP-13C	Nucleosides, Nucleotides, and Analogues	2.65E+07	2.51E+07	2.75E+07	2.81E+07	2.35E+07	7.14%	24.66003333	24.58175869	24.7134528	24.74506622	24.4867712	0.42%
Arginine-13C	Amino Acids and Derivatives	1.30E+07	1.35E+07	1.21E+07	1.30E+07	1.35E+07	4.40%	23.63644053	23.6907244	23.53326509	23.62644876	23.6907244	0.27%
Ascorbic acid-13C	Organic acids	3.89E+07	3.82E+07	3.80E+07	3.79E+07	3.82E+07	0.96%	25.21141126	25.18517972	25.17987569	25.17607512	25.18744692	0.05%
Asparagine-13C	Amino Acids and Derivatives	3.01E+07	3.14E+07	3.10E+07	3.33E+07	3.32E+07	4.49%	24.84182153	24.90288219	24.88436805	24.98945202	24.98511439	0.26%
Aspartic acid-13C	Amino Acids and Derivatives	8.91E+05	8.94E+05	9.00E+05	8.86E+05	8.73E+05	1.15%	19.76441809	19.76926966	19.77892414	19.7562957	19.73496095	0.08%
ATP-13C	Nucleosides, Nucleotides, and Analogues	5.74E+07	5.61E+07	5.51E+07	5.94E+07	5.42E+07	3.57%	25.77354169	25.74124025	25.71554898	25.82298776	25.69221534	0.20%
Benzoic acid-13C	Organic acids	6.57E+06	6.49E+06	6.69E+06	6.50E+06	6.53E+06	1.24%	22.64812055	22.63045378	22.67422132	22.63223022	22.63931421	0.08%
Beta-alanine-13C	Amino Acids and Derivatives	1.73E+05	1.77E+05	1.63E+05	1.33E+05	1.70E+05	10.94%	17.39623684	17.43420469	17.31008019	17.01563283	17.37602362	0.97%
Carbamoyl-phosphate-13C	Organic Phosphate	1.67E+06	1.60E+06	1.53E+06	1.58E+06	1.68E+06	3.91%	20.67141667	20.60964047	20.54510022	20.59149313	20.6800298	0.27%
CDP-13C	Nucleosides, Nucleotides, and Analogues	7.69E+06	7.71E+06	7.60E+06	7.45E+06	7.82E+06	1.81%	22.87455217	22.87829943	22.85756799	22.82880899	22.89873718	0.11%
Choline-13C	Alcohols and Polyols	2.91E+07	2.86E+07	2.93E+07	2.96E+07	2.81E+07	2.03%	24.79302774	24.77052034	24.80291941	24.81763091	24.74252573	0.12%
Citric acid-13C	Organic acids	2.93E+08	2.91E+08	2.86E+08	2.73E+08	2.86E+08	2.72%	28.1248475	28.11396292	28.09194426	28.02273946	28.0889155	0.14%
Citulline-13C	Amino Acids and Derivatives	4.46E+06	4.42E+06	4.36E+06	4.41E+06	4.41E+06	2.14%	22.08764153	22.0746354	22.05490368	22.07136547	22.13539617	0.14%
CMP-13C	Nucleosides, Nucleotides, and Analogues	7.64E+05	7.84E+05	7.04E+05	7.69E+05	7.34E+05	4.25%	19.54283539	19.58012605	19.42480599	19.55224881	19.48502738	0.32%
Coenzyme A-13C	Cofactors	6.51E+05	6.31E+05	6.43E+05	6.11E+05	6.44E+05	2.47%	19.31207639	19.26819474	19.29333693	19.22010432	19.29647712	0.19%
CTP-13C	Nucleosides, Nucleotides, and Analogues	1.92E+06	1.88E+06	1.97E+06	1.78E+06	1.90E+06	3.64%	20.8891296	20.83997722	20.91049635	20.76587527	20.85680847	0.25%
cyclic AMP-13C	Nucleosides, Nucleotides, and Analogues	1.47E+06	1.39E+06	1.40E+06	1.54E+06	1.43E+06	4.16%	20.48246923	20.40145455	20.41802553	20.54980722	20.44253049	0.29%
Cystathionine-13C	Amino Acids and Derivatives	2.51E+04	2.59E+04	2.18E+04	2.61E+04	2.01E+04	11.36%	14.61424973	14.65955	14.41071633	14.6720938	14.29347165	1.16%
Cysteine-13C	Amino Acids and Derivatives	3.06E+04	3.16E+04	3.08E+04	3.15E+04	3.36E+04	3.75%	14.89888476	14.94535238	14.90923682	14.9407724	15.03402515	0.36%
Cytidine-13C	Nucleosides, Nucleotides, and Analogues	2.06E+05	2.19E+05	2.21E+05	1.86E+05	2.34E+05	8.51%	17.65298498	17.74122996	17.7543395	17.50571853	17.83676541	0.71%
Cytosine-13C	Nucleosides, Nucleotides, and Analogues	1.45E+06	1.42E+06	1.43E+06	1.55E+06	1.35E+06	5.02%	20.46363612	20.43338983	20.44556455	20.56010889	20.36024698	0.35%
dADP-13C	Nucleosides, Nucleotides, and Analogues	1.37E+06	1.31E+06	1.30E+06	1.26E+06	1.38E+06	3.92%	20.38152605	20.31672347	20.30563429	20.26040503	20.39728189	0.28%
dAMP-13C	Nucleosides, Nucleotides, and Analogues	3.42E+05	3.02E+05	3.65E+05	3.36E+05	3.52E+05	6.96%	18.38405858	18.20466666	18.47793214	18.35853102	18.4256257	0.56%
dATP-13C	Nucleosides, Nucleotides, and Analogues	1.14E+05	1.31E+05	1.17E+05	1.07E+05	1.32E+05	9.02%	16.80372753	17.00140819	16.83368075	16.71263447	17.01127094	0.77%
dCDP-13C	Nucleosides, Nucleotides, and Analogues	8.70E+06	8.03E+06	8.59E+06	8.62E+06	8.79E+06	3.49%	23.05274979	22.93714821	23.03372276	23.03942379	23.06759585	0.22%
dCMP-13C	Nucleosides, Nucleotides, and Analogues	1.15E+05	1.35E+05	1.25E+05	1.10E+05	1.18E+05	7.94%	16.8162837	17.04366815	16.93617782	16.75238065	16.85330956	0.67%
dCTP-13C	Nucleosides, Nucleotides, and Analogues	2.28E+06	2.33E+06	2.22E+06	2.52E+06	2.41E+06	4.98%	21.11996949	21.15127921	21.08147824	21.26441969	21.20606172	0.34%
Deoxyadenosine-13C	Nucleosides, Nucleotides, and Analogues	7.42E+05	7.38E+05	7.40E+05	7.30E+05	7.32E+05	0.71%	19.50086521	19.49345676	19.49736069	19.47714163	19.48128702	0.05%
Deoxyguanosine-13C	Nucleosides, Nucleotides, and Analogues	1.68E+06	1.71E+06	1.61E+06	1.57E+06	1.64E+06	3.41%	20.68174627	20.70725127	20.6177329	20.58416979	20.64085921	0.24%
Deoxyinosine-13C	Nucleosides, Nucleotides, and Analogues	2.14E+05	1.84E+05	2.06E+05	2.18E+05	2.21E+05	7.14%	17.70522738	17.4869921	17.65018227	17.73198188	17.75238065	0.60%
Deoxyribose phosphate-13C	Sugar and Sugar Phosphate	8.09E+04	8.12E+04	8.21E+04	7.80E+04	7.99E+04	1.95%	16.30385208	16.30919211	16.3250946	16.2511865	16.28590788	0.17%
Deoxyuridine-13C	Nucleosides, Nucleotides, and Analogues	3.69E+05	3.61E+05	3.59E+05	3.54E+05	3.19E+05	5.52%	18.49208789	18.4604399	18.45241822	18.43216669	18.28183949	0.45%
Deoxyphospho-CoA-13C	Cofactors	1.88E+05	1.75E+05	1.80E+05	1.79E+05	1.69E+05	4.00%	17.52267347	17.41946647	17.46003987	17.45201596	17.36521176	0.33%
dGDP-13C	Nucleosides, Nucleotides, and Analogues	2.37E+05	2.31E+05	2.07E+05	2.64E+05	2.44E+05	8.75%	17.85330956	17.8162837	17.65787666	18.00908504	17.8953386	0.72%
dGMP-13C	Nucleosides, Nucleotides, and Analogues	5.63E+05	5.12E+05	5.71E+05	5.66E+05	5.61E+05	4.35%	19.1027754	18.96578428	19.12313122	19.11044253	19.09764125	0.34%
dGTP-13C	Nucleosides, Nucleotides, and Analogues	3.76E+05	3.70E+05	3.56E+05	3.86E+05	3.71E+05	2.90%	18.5219071	18.49755561	18.44313781	18.5861503	18.50067074	0.23%
Dihydrofolic acid-13C	Vitamins and Derivatives	3.07E+04	2.47E+04	2.57E+04	2.87E+04	2.77E+04	8.69%	14.90454055	14.5904701	14.64779568	14.80725428	14.75603502	0.35%
dIMP-13C	Nucleosides, Nucleotides, and Analogues	2.38E+06	2.05E+06	2.73E+06	2.54E+06	2.78E+06	11.85%	21.18313619	20.96789606	21.38152605	21.2766946	21.40717231	0.84%
dITP-13C	Nucleosides, Nucleotides, and Analogues	5.02E+04	5.32E+04	4.92E+04	5.16E+04	4.82E+04	3.95%	15.61424973	15.69949112	15.5851973	15.65396464	15.5554777	0.36%
dTDP-13C	Nucleosides, Nucleotides, and Analogues	9.45E+04	1.19E+05	9.95E+04	8.94E+04	9.45E+04	11.81%	16.52741592	16.86592655	16.60182881	16.44734157	16.52741592	0.97%
dTDP-D-Glucose-13C	Nucleosides, Nucleotides, and Analogues	4.33E+05	4.25E+05	4.03E+05	4.16E+05	4.23E+05	2.68%	18.7240075	18.69710332	18.62042031	18.666224	18.68859182	0.2

Gamma-Aminobutyric acid-13C	Amino Acids and Derivatives	8.60E+05	8.20E+05	7.60E+05	8.10E+05	8.04E+05	4.42%	19.71313811	19.64438442	19.53469044	19.62667155	19.6159385	0.33%
GDP-13C	Nucleosides, Nucleotides, and Analogues	1.73E+06	1.78E+06	1.69E+06	1.82E+06	1.92E+06	4.81%	20.72484022	20.76587527	20.69115054	20.79788313	20.86966613	0.33%
Geranyl-PP-13C	Organic phosphate	4.40E+04	4.52E+04	4.20E+04	4.61E+04	4.51E+04	3.57%	15.42390377	15.46275787	15.35672706	15.49247913	15.46083981	0.34%
Glucaric acid-13C	Organic acids	2.04E+06	2.36E+06	2.54E+06	2.44E+06	2.16E+06	8.88%	20.95801455	21.16852033	21.27469209	21.21667482	21.04059475	0.61%
Gluconic acid-13C	Organic acids	5.22E+06	5.52E+06	5.02E+06	4.72E+06	5.12E+06	5.69%	22.1644727	22.3970207	22.26011784	22.1712721	22.28855746	0.37%
Glucosamine 6-phosphate-13C	Sugar and Sugar Phosphate	2.89E+05	2.83E+05	2.92E+05	2.75E+05	2.88E+05	2.34%	18.14021068	18.10993265	18.15610283	18.06907209	18.13621013	0.19%
Glucosamine-13C	Sugar and Sugar Phosphate	3.63E+05	3.60E+05	3.41E+05	3.59E+05	3.73E+05	3.18%	18.46841722	18.45803807	18.37983523	18.45402613	18.50765529	0.25%
Glutaconic acid-13C	Organic acids	1.80E+07	1.89E+07	1.81E+07	1.73E+07	1.65E+07	5.09%	24.10149357	24.1718829	24.10948636	24.0442687	23.97596269	0.31%
Glutamic acid-13C	Amino Acids and Derivatives	1.72E+07	1.84E+07	1.77E+07	1.76E+07	1.73E+07	2.64%	24.0333867	24.13084829	24.07316485	24.06661086	24.04510239	0.16%
Glutamine-13C	Amino Acids and Derivatives	1.79E+06	1.89E+06	1.75E+06	1.73E+06	1.75E+06	3.61%	20.76991531	20.84842733	20.73727375	20.72067179	20.73727375	0.25%
Glyceraldehyde 3-phosphate-13C	Organic phosphate	5.70E+05	5.76E+05	5.61E+05	5.78E+05	5.48E+05	2.19%	19.11984288	19.13495769	19.09686954	19.14095955	19.06328974	0.17%
Glyceraldehyde-13C	Alcohols and Polyols	1.96E+05	1.90E+05	2.26E+05	1.89E+05	1.99E+05	7.55%	17.58049413	17.53563989	17.78596325	17.52878984	17.60240891	0.60%
Glyceric acid-13C	Organic acids	3.81E+06	3.71E+06	3.79E+06	3.64E+06	3.89E+06	2.63%	21.86287341	21.82454238	21.85528825	21.79352393	21.89282145	0.17%
Glycerol 3-phosphate-13C	Organic Phosphate	6.42E+06	6.12E+06	6.31E+06	6.02E+06	6.51E+06	3.26%	22.61369236	22.54462868	22.59012283	22.52085268	22.63422611	0.21%
Glycerol-13C	Alcohols and Polyols	5.17E+04	5.34E+04	5.36E+04	5.47E+04	5.21E+04	2.27%	15.65676002	15.70401169	15.71021451	15.73819784	15.66954946	0.21%
Glycerophosphocholine-13C	Alcohols and Polyols	1.05E+06	1.35E+06	1.25E+06	1.15E+06	1.22E+06	9.31%	20.00333124	20.3659624	20.25465036	20.1344564	20.21963177	0.67%
Glycine-13C	Amino Acids and Derivatives	8.90E+05	8.80E+05	8.95E+05	8.86E+05	8.70E+05	1.10%	19.7636079	19.74730793	19.77168934	19.75711	19.73049004	0.08%
Glycolic acid-13C	Organic acids	2.55E+06	2.50E+06	2.52E+06	2.45E+06	2.62E+06	2.50%	21.2831969	21.25465036	21.26613684	21.22552755	21.32278638	0.17%
Glyoxylic acid-13C	Organic acids	6.14E+05	6.27E+05	6.10E+05	6.12E+05	6.11E+05	1.13%	19.22858386	19.25879604	19.21915906	19.22387916	19.22152104	0.08%
GMP-13C	Nucleosides, Nucleotides, and Analogues	1.58E+06	1.63E+06	1.50E+06	1.50E+06	1.63E+06	4.14%	20.58966577	20.63820963	20.51460619	20.51749255	20.63200829	0.29%
GTP-13C	Nucleosides, Nucleotides, and Analogues	7.63E+05	7.62E+05	7.83E+05	7.50E+05	7.69E+05	1.57%	19.54056701	19.53867395	19.57791558	19.51576143	19.55187345	0.12%
Guanine-13C	Nucleosides, Nucleotides, and Analogues	7.23E+05	7.48E+05	6.93E+05	7.03E+05	7.52E+05	3.65%	19.46343656	19.51248586	19.40228763	19.42295993	19.52094856	0.27%
Guanosine-13C	Nucleosides, Nucleotides, and Analogues	5.86E+06	5.92E+06	5.80E+06	5.72E+06	5.63E+06	1.98%	22.48246923	22.49740942	22.46726147	22.44758372	22.42470349	0.13%
Hexose biphosphate-13C	Sugar and Sugar Phosphate	2.13E+07	2.11E+07	2.06E+07	2.10E+07	2.15E+07	1.53%	24.34163826	24.3280021	24.296141	24.32251134	24.35514674	0.09%
Hexose monophosphate-13C	Sugar and Sugar Phosphate	6.43E+07	6.39E+07	6.40E+07	6.36E+07	6.40E+07	0.40%	25.93809011	25.9290868	25.93089215	25.92206968	25.93179397	0.02%
Hexose pool-13C	Sugar and Sugar Phosphate	3.57E+08	3.29E+08	3.51E+08	3.22E+08	3.49E+08	4.46%	28.41094466	28.29351234	28.3877176	28.26203734	28.37823836	0.23%
Histidine-13C	Amino Acids and Derivatives	9.00E+05	8.80E+05	9.10E+05	9.50E+05	8.10E+05	5.78%	19.7798604	19.74747185	19.79582406	19.85787168	19.62791856	0.43%
Homocysteine-13C	Amino Acids and Derivatives	4.31E+04	4.01E+04	3.92E+04	4.21E+04	4.52E+04	5.71%	15.3943957	15.29023489	15.25746151	15.36084708	15.46307729	0.53%
Homoserine-13C	Amino Acids and Derivatives	7.60E+05	7.57E+05	7.49E+05	7.68E+05	7.70E+05	1.15%	19.53620927	19.5305054	19.51364279	19.55131023	19.55449892	0.08%
Hydroxyphenyllactic acid-13C	Organic acids	3.00E+05	3.20E+05	3.42E+05	2.82E+05	2.91E+05	7.93%	18.19219648	18.28545641	18.38405858	18.1027754	18.14817864	0.62%
Hypoxanthine-13C	Nucleosides, Nucleotides, and Analogues	3.76E+05	3.61E+05	3.83E+05	3.89E+05	3.70E+05	2.90%	18.5219071	18.46323698	18.5473615	18.57089336	18.49872457	0.23%
IDP-13C	Nucleosides, Nucleotides, and Analogues	3.94E+04	3.85E+04	4.22E+04	3.86E+04	3.82E+04	4.13%	15.2644426	15.23406895	15.36358725	15.23481743	15.21977355	0.38%
IMP-13C	Nucleosides, Nucleotides, and Analogues	2.31E+05	2.44E+05	2.36E+05	2.46E+05	2.16E+05	5.15%	17.81565848	17.89593023	17.84659223	17.90653833	17.71866665	0.42%
Inosine-13C	Nucleosides, Nucleotides, and Analogues	4.83E+05	4.75E+05	4.60E+05	4.89E+05	4.92E+05	2.68%	18.88255947	18.85817531	18.81221492	18.90065458	18.90917821	0.21%
Isoleucine-13C	Amino Acids and Derivatives	4.20E+07	4.22E+07	4.10E+07	4.13E+07	4.30E+07	1.93%	25.32216747	25.33176491	25.28736012	25.29963845	25.35850419	0.11%
ITP-13C	Nucleosides, Nucleotides, and Analogues	2.53E+06	2.14E+06	2.30E+06	2.76E+06	2.51E+06	9.73%	21.27241565	21.02917937	21.13257504	21.39780413	21.25810592	0.67%
Lactic acid-13C	Organic acids	2.65E+06	2.61E+06	2.59E+06	2.61E+06	2.72E+06	1.92%	21.33483629	21.31285194	21.30507758	21.31285194	21.37252077	0.13%
Leucine-13C	Amino Acids and Derivatives	6.50E+05	6.29E+05	6.22E+05	6.20E+05	6.05E+05	2.61%	19.30919211	19.26178275	19.24539487	19.24097762	19.20648023	0.19%
Lysine-13C	Amino Acids and Derivatives	1.53E+05	1.57E+05	1.42E+05	1.50E+05	1.62E+05	4.80%	17.22599817	17.26315915	17.11857614	17.19748548	17.30296015	0.41%
LysoPC(16:0)-13C	Phospholipids	2.70E+06	2.76E+06	2.82E+06	2.61E+06	2.60E+06	3.52%	21.36292409	21.39466784	21.42572813	21.31395915	21.30841458	0.24%
LysoPC(18:0)-13C	Phospholipids	1.12E+07	1.33E+07	1.21E+07	1.20E+07	1.02E+07	9.81%	23.41312585	23.66166503	23.52492234	23.51291982	23.27781634	0.61%
LysoPC(22:0)-13C	Phospholipids	6.33E+04	6.11E+04	6.35E+04	6.43E+04	6.31E+04	1.89%	15.94923398	15.89817622	15.9551504	15.97185785	15.94466631	0.17%
Malic acid-13C	Organic acids	1.28E+07	1.27E+07	1.21E+07	1.32E+07	1.30E+07	3.27%	23.60625519	23.59263405	23.65512713	23.65512713	23.62867514	0.20%
Malonyl-CoA-13C	Cofactors	2.86E+05	2.06E+05	2.30E+05	2.45E+05	2.86E+05	14.03%	18.12464639	17.65088346	17.81064694	17.90418771	18.12464639	1.14%
Methionine-13C	Amino Acids and Derivatives	7.26E+06	7.13E+06	7.32E+06	7.41E+06	7.20E+06	1.48%	22.79114063	22.76506591	22.80242643	22.82065267	22.77956548	0.09%
Myoinositol-13C	Sugar and Sugar Phosphate	7.75E+04	7.60E+04	7.15E+04	7.35E+04	7.21E+04	3.46%	16.24209483	16.21390161	16.12585738	16.1656529	16.13791172	0.31%
N-Acetyl-glucosamine 1-phosphate-13C	Sugar and Sugar Phosphate	3.13E+05	3.10E+05	3.21E+05	3.36E+05	3.41E+05	4.20%	18.25718524	18.24330417	18.29266314	18.35681301	18.38025812	0.33%
N-Acetylornithine-13C	Amino Acids and Derivatives	4.70E+05	4.76E+05	4.00E+05	3.90E+05	4.00E+05	9.84%	18.84352853	18.86181389	18.61108245	18.57459353	18.61108245	0.75%
N-acetyls erine-13C	Amino Acids and Derivatives	1.32E+07	1.43E+07	1.36E+07	1.02E+07	1.28E+07	12.24%	23.65075201	23.766482	23.69391738	23.7781634	23.61076714	0.80%
NAD+13C	Nucleosides, Nucleotides, and Analogues	2.08E+05	2.39E+05	2.21E+05	1.90E+05	2.13E+05	8.37%	17.66761054	17.86785786	17.7562957	17.53715772	17.70184791	0.68%
NADH-13C	Nucleosides, Nucleotides, and Analogues	3.48E+06	3.62E+06	3.18E+06	3.28E+06	3.20E+06	5.70%	21.73189904	21.78795675	21.60195573	21.64658332	21.60918956	0.38%
NADP+13C	Nucleosides, Nucleotides, and Analogues	1.35E+06	1.42E+06	1.39E+06	1.25E+06	1.15E+06	8.45%	20.36559624	20.43847512	20.40769099	20.25465036	20.1344564	0.62%
NADPH-13C	Nucleosides, Nucleotides, and Analogues	4.14E+06	4.18E+06	4.33E+06	4.26E+06	4.04E+06	2.66%	21.9794559	21.99541661	22.0442687	22.02106672	21.94413724	0.17%
Niacinamide-13C	Vitamins and Derivatives	2.10E+06	2.07E+06	2.15E+06	2.22E+06	2.18E+06	2.82%	21.00333124	20.97910696	21.03724665	21.08082793	21.05655834	0.19%
Nicotinic acid-13C	Vitamins and Derivatives	3.02E+06	3.32E+06	3.32E+06	3.14E+06	2.92E+06	5.68%	21.52563933	21.6623172	21.6623172	21.58141392	21.47704278	0.38%
Oleic acid-13C	Phospholipids	4.52E+04	4.32E+04	4.42E+04	4.59E+04	4.72E+04	3.39%	15.46499238	15.39974522	15.43273762	15.48463411	15.52741592	0.32%
Ornithine-13C	Amino Acids and Derivatives	6.03E+05	6.73E+05	6.28E+05	6.15E+05	5.93E+05	5.01%	19.20084115	19.35938925	19.26040503	19.23046145	19.1766991	0.37%
Orotidyl acid-13C	Nucleosides, Nucleotides, and Analogues	7.31E+04	7.35E+04	7.26E+04	7.25E+04	7.08E+04	1.43%	16.15738641	16.1656529	16.14780565	16.14648912	16.11125795	0.13%
Oxalic acid-13C	Organic acids	3.74E+06	3.64E+06	3.94E+06	3.65E+06	3.79E+06	3.25%	21.83383514	21.79471411	21.90903168	21.79986024	21.85414703	0.21%
Oxaloacetic acid-13C	Organic acids	8.83E+05	8.95E+05	8.91E+05	8.37E+05	8.69E+05	2.67%	19.75270731	19.77217279	19.76506591	19.67555739	19.72966057	0.20%
Oxidized glutathione-13C	Amino Acids and Derivatives	6.58E+05	6.73E+05	6.62E+05	6.54E+05	6.78E+05	1.54%	19.32750879	19.3600326	19.33625375	19.31782771	19.37071295	0.11%
Oxoglutaric acid-13C	Organic acids	1.25E+07	1.24E+07	1.20E+07	1.27E+07	1.22E+07	2.18%	23.57657845	23.56499978	23.57177382	23.59832516	23.53919479	0.13%
PA(28:0)-13C	Phospholipids	1.96E+05	2.26E+05	2.00E+05	1.91E+05	2.16E+05	7.14%	17.57872648	17.78443037	17.6079082	17.54139916	17.7190679	0.58%
PA(28:1)-13C	Phospholipids	5.23E+05	5.19E+05	5.20E+05	5.35E+05	5.40E+05	1.84%	18.99727873	18.98454084	18.98676422	19.029449	19.04286702	0.14%

PC(24:0)-13C	Phospholipids	1.40E+07	1.39E+07	1.42E+07	1.45E+07	1.38E+07	2.06%	23.74201167	23.72546445	23.76243233	23.79253137	23.72025428	0.12%
PC(24:1)-13C	Phospholipids	2.29E+06	2.15E+06	2.15E+06	2.32E+06	2.22E+06	3.47%	21.12439397	21.03657609	21.03321865	21.14320382	21.07952645	0.24%
PC(26:0)-13C	Phospholipids	1.43E+07	1.41E+07	1.47E+07	1.46E+07	1.33E+07	3.93%	23.76547065	23.74509326	23.80538177	23.79550702	23.66057744	0.24%
PC(26:1)-13C	Phospholipids	2.45E+07	2.39E+07	2.25E+07	2.48E+07	2.31E+07	4.05%	24.54863191	24.50869523	24.42598418	24.56616184	24.46138952	0.24%
PC(28:0)-13C	Phospholipids	6.67E+06	6.65E+06	6.77E+06	6.90E+06	6.48E+06	2.31%	22.66882267	22.66579044	22.69029814	22.7177467	22.62711704	0.15%
PC(28:1)-13C	Phospholipids	9.27E+05	9.56E+05	8.87E+05	8.77E+05	9.07E+05	3.50%	19.82189852	19.86680199	19.75824924	19.74188827	19.79042487	0.25%
PC(28:2)-13C	Phospholipids	6.00E+06	5.76E+06	5.80E+06	6.20E+06	6.10E+06	3.16%	22.51605009	22.45713636	22.46787019	22.56337132	22.53990472	0.20%
PC(30:0)-13C	Phospholipids	9.28E+06	9.21E+06	9.18E+06	9.23E+06	9.19E+06	0.43%	23.14522691	23.13429972	23.12959118	23.1385243	23.13163343	0.03%
PC(30:1)-13C	Phospholipids	5.47E+06	5.41E+06	5.38E+06	5.52E+06	5.26E+06	1.80%	22.3836368	22.36693047	22.35944288	22.39519103	22.32690562	0.12%
PC(30:2)-13C	Phospholipids	1.57E+07	1.63E+07	1.61E+07	1.59E+07	1.49E+07	3.38%	23.90701533	23.96013772	23.94055735	23.92524293	23.83171083	0.21%
PC(32:0)-13C	Phospholipids	1.12E+06	1.10E+06	1.02E+06	1.25E+06	1.17E+06	7.51%	20.0989265	20.07300136	19.96437471	20.25695498	20.16177158	0.54%
PC(32:1)-13C	Phospholipids	9.55E+05	9.62E+05	9.51E+05	9.49E+05	9.32E+05	1.16%	19.86453681	19.87582733	19.85878238	19.85635257	19.83012522	0.08%
PC(32:2)-13C	Phospholipids	1.12E+06	1.02E+06	1.32E+06	1.09E+06	1.12E+06	9.83%	20.0899056	19.95446897	20.32772806	20.0558967	20.09377861	0.68%
PC(34:1)-13C	Phospholipids	3.50E+06	3.42E+06	3.33E+06	3.56E+06	3.64E+06	3.46%	21.73686102	21.70345415	21.66492291	21.76141813	21.79352393	0.23%
PC(34:2)-13C	Phospholipids	7.12E+06	7.24E+06	6.98E+06	6.87E+06	7.21E+06	2.21%	22.76344581	22.78755827	22.73479561	22.71187867	22.78156783	0.14%
PC(36:0)-13C	Phospholipids	7.41E+05	7.38E+05	7.32E+05	7.43E+05	7.22E+05	1.18%	19.49814021	19.49345676	19.48049834	19.50339098	19.46063987	0.09%
PC(36:1)-13C	Phospholipids	1.15E+07	1.25E+07	1.11E+07	1.17E+07	1.18E+07	4.37%	23.45387546	23.57427014	23.40275603	23.47877159	23.49106038	0.27%
PC(36:2)-13C	Phospholipids	1.81E+07	1.88E+07	1.78E+07	1.91E+07	1.78E+07	3.15%	24.11107962	24.16269373	24.08618418	24.18555784	24.08790337	0.19%
PC(36:4)-13C	Phospholipids	7.91E+05	7.95E+05	8.01E+05	8.31E+05	7.71E+05	2.72%	19.59350055	19.60077679	19.61162282	19.66466255	19.55655844	0.20%
PC(38:3)-13C	Phospholipids	5.21E+05	5.28E+05	5.32E+05	5.01E+05	5.32E+05	2.47%	18.98981579	19.00908504	19.02133788	18.93445108	19.02025294	0.19%
PC(38:5)-13C	Phospholipids	8.66E+04	8.53E+04	8.81E+04	8.69E+04	8.52E+04	1.40%	16.40274562	16.38059635	16.42750928	16.40773248	16.37924297	0.12%
PE(28:0)-13C	Phospholipids	1.80E+06	1.87E+06	1.67E+06	1.71E+06	1.83E+06	4.77%	20.77876376	20.83383514	20.67055252	20.70134031	20.80420036	0.33%
PE(28:1)-13C	Phospholipids	5.65E+06	5.05E+06	5.71E+06	5.61E+06	5.83E+06	5.42%	22.43084045	22.26899423	22.44606961	22.42059763	22.47605396	0.36%
PE(30:0)-13C	Phospholipids	1.64E+05	1.60E+05	1.71E+05	1.60E+05	1.66E+05	2.80%	17.3250946	17.28951462	17.38532318	17.28951462	17.34256086	0.23%
PE(30:1)-13C	Phospholipids	5.25E+05	5.21E+05	5.33E+05	5.46E+05	5.23E+05	1.93%	19.00140819	18.99092385	19.02323456	19.05801287	18.9958962	0.15%
PE(30:2)-13C	Phospholipids	1.12E+06	1.22E+06	1.11E+06	1.19E+06	1.14E+06	4.14%	20.09119776	20.21489774	20.07952645	20.18374198	20.11680082	0.29%
PE(32:1)-13C	Phospholipids	4.24E+05	4.21E+05	4.20E+05	4.33E+05	4.20E+05	1.36%	18.69234306	18.68208932	18.67865515	18.72500671	18.67934264	0.10%
PE(32:2)-13C	Phospholipids	3.50E+05	3.61E+05	3.71E+05	3.38E+05	3.41E+05	3.93%	18.41658314	18.46203889	18.50105966	18.36709049	18.37898907	0.31%
PE(34:1)-13C	Phospholipids	9.34E+05	9.22E+05	9.28E+05	9.27E+05	9.31E+05	0.48%	19.83229905	19.81362464	19.82423159	19.82236544	19.82764662	0.03%
PE(34:2)-13C	Phospholipids	6.49E+05	6.41E+05	6.38E+05	6.67E+05	6.39E+05	1.87%	19.30674705	19.28883905	19.28062582	19.34624535	19.28432709	0.14%
PE(36:1)-13C	Phospholipids	7.06E+05	6.86E+05	6.16E+05	7.16E+05	7.36E+05	6.67%	19.42849104	19.38700758	19.23163371	19.44879386	19.48856195	0.51%
PE(36:2)-13C	Phospholipids	4.66E+06	4.06E+06	4.19E+06	4.67E+06	4.86E+06	7.66%	22.15189852	21.9530483	21.99851881	22.15499112	22.21252488	0.51%
PG(32:1)-13C	Phospholipids	9.72E+05	9.70E+05	9.65E+05	9.80E+05	9.91E+05	1.05%	19.89000296	19.88688137	19.88046839	19.90212777	19.91881666	0.08%
PG(32:2)-13C	Phospholipids	2.81E+06	2.75E+06	2.66E+06	2.85E+06	2.77E+06	2.65%	21.42367812	21.39257318	21.34245235	21.4445539	21.40301619	0.18%
PG(34:1)-13C	Phospholipids	8.72E+05	8.70E+05	8.65E+05	8.79E+05	8.45E+05	1.49%	19.73446486	19.73115327	19.72840888	19.74599594	19.68910392	0.11%
PG(34:2)-13C	Phospholipids	3.05E+05	3.35E+05	2.85E+05	3.13E+05	2.89E+05	6.59%	18.21844972	18.35380157	18.20602039	18.25580313	18.14070997	0.52%
Phenylalanine-13C	Amino Acids and Derivatives	2.46E+08	2.25E+08	2.38E+08	2.44E+08	2.16E+08	5.52%	27.87349649	27.74631599	27.82335227	27.86230591	27.68445094	0.29%
Phenylactic acid-13C	Organic acids	4.70E+05	4.77E+05	4.72E+05	4.83E+05	4.71E+05	1.19%	18.84076563	18.86211669	18.84689825	18.88224633	18.84444833	0.09%
Phenylpyruvic acid-13C	Organic acids	3.57E+05	3.49E+05	3.72E+05	3.65E+05	3.41E+05	3.45%	18.44475609	18.41286751	18.50416724	18.4767462	18.37856581	0.27%
Phosphoenolpyruvic acid-13C	Organic Phosphate	3.11E+07	3.08E+07	3.32E+07	3.16E+07	3.20E+07	2.89%	24.89133872	24.87689535	24.98294067	24.91250784	24.93201934	0.17%
Phosphoribosyl pyrophosphate-13C	Organic phosphate	4.37E+04	4.51E+04	4.49E+04	4.67E+04	4.05E+04	5.24%	15.4166656	15.4621188	15.4557125	15.51237011	15.3705847	0.50%
Phosphorylcholine-13C	Alcohols and Polyols	1.94E+06	1.92E+06	1.91E+06	1.92E+06	1.90E+06	0.73%	20.88467452	20.86991296	20.86362974	20.8753774	20.85756799	0.05%
Phosphoserine-13C	Organic phosphate	4.60E+05	4.51E+05	4.44E+05	4.72E+05	4.56E+05	2.30%	18.81096067	18.78244798	18.75987518	18.84812165	18.79835788	0.18%
PI(26:0)-13C	Phospholipids	1.33E+06	1.33E+06	1.33E+06	1.33E+06	1.33E+06	0.00%	20.34516265	20.34516265	20.34516265	20.34516265	20.34516265	0.00%
PI(28:0)-13C	Phospholipids	3.92E+05	4.12E+05	3.52E+05	3.72E+05	3.85E+05	5.85%	18.58196552	18.65368481	18.4268544	18.50649355	18.55599705	0.46%
PI(28:1)-13C	Phospholipids	2.01E+06	2.34E+06	2.10E+06	1.91E+06	2.21E+06	7.95%	20.93589018	21.15560884	21.00470327	20.86211669	21.07300136	0.55%
PI(30:0)-13C	Phospholipids	2.49E+05	2.53E+05	2.55E+05	2.62E+05	2.40E+05	3.22%	19.92752336	19.95048755	19.96183401	18.00085828	17.87447712	0.26%
PI(30:1)-13C	Phospholipids	2.13E+05	2.11E+05	2.23E+05	2.31E+05	2.26E+05	3.95%	17.69846051	17.68483079	17.76474203	17.81878187	17.78404689	0.32%
PI(30:2)-13C	Phospholipids	4.66E+05	4.60E+05	4.56E+05	4.69E+05	4.62E+05	1.10%	18.83027999	18.81158793	18.79899064	18.83953598	18.81784556	0.08%
PI(32:0)-13C	Phospholipids	5.20E+05	5.32E+05	5.11E+05	5.21E+05	5.33E+05	1.70%	18.98676422	19.01971017	18.9638105	18.99092385	19.022422	0.13%
PI(32:1)-13C	Phospholipids	8.04E+05	8.13E+05	7.94E+05	7.84E+05	7.64E+05	2.39%	19.61737419	19.63342809	19.59932448	19.58104607	19.5437795	0.18%
PI(32:2)-13C	Phospholipids	7.68E+04	7.70E+04	7.54E+04	7.49E+04	7.74E+04	1.41%	16.22806709	16.23182118	16.20151134	16.1926781	16.23930017	0.13%
PI(34:1)-13C	Phospholipids	4.08E+04	3.88E+04	4.18E+04	4.18E+04	4.00E+04	3.15%	15.31451244	15.24190869	15.34948858	15.35052487	15.28699085	0.30%
PI(34:2)-13C	Phospholipids	1.30E+06	1.45E+06	1.34E+06	1.29E+06	1.27E+06	5.47%	20.31340565	20.46861609	20.35702787	20.29333693	20.27639707	0.38%
PI(36:2)-13C	Phospholipids	1.60E+06	1.63E+06	1.56E+06	1.47E+06	1.39E+06	6.45%	20.61144272	20.63820963	20.57496302	20.48934624	20.40872778	0.46%
PI(36:1)-13C	Phospholipids	6.52E+04	6.49E+04	6.40E+04	6.41E+04	6.21E+04	1.84%	15.99168998	15.98526382	15.96533337	15.96848681	15.92323462	0.17%
PI(36:2)-13C	Phospholipids	3.00E+05	3.18E+05	2.76E+05	2.92E+05	3.10E+05	5.39%	18.19219648	18.27639707	18.07430874	18.15313636	18.23957988	0.43%
Prephenate-13C	Organic acids	2.23E+06	2.17E+06	2.20E+06	2.15E+06	2.27E+06	2.15%	21.08925908	21.05125674	21.06972771	21.03657609	21.11489628	0.15%
Proline-13C	Amino Acids and Derivatives	2.29E+06	2.21E+06	2.39E+06	2.05E+06	2.27E+06	5.59%	21.12817561	21.07691995	21.18978596	20.9685993	21.1155314	0.39%
Propionyl-CoA-13C	Cofactors	1.79E+05	1.52E+05	1.59E+05	1.63E+05	1.71E+05	6.37%	17.44879386	17.21276234	17.2777596	17.31362708	17.38279287	0.53%
PS(32:0)-13C	Phospholipids	7.75E+04	7.65E+04	7.51E+04	7.85E+04	7.43E+04	2.25%	16.24209483	16.22317213	16.19614103	16.2605888	16.18126875	0.20%
PS(32:1)-13C	Phospholipids	1.20E+05	1.23E+05	1.33E+05	1.50E+05	1.33E+05	8.93%	16.86785786	16.90359945	17.01672125	17.19075065	17.01672125	0.74%
PS(32:2)-13C	Phospholipids	3.23E+05	3.20E+05	3.13E+05	3.27E+05	3.20E+05	1.60%	18.30251398	18.28906427	18.25718524	18.32025408	18.28726147	0.13%
PS(34:1)-13C	Phospholipids	6.84E+04	6.89E+04	6.75E+04	6.68E+04	6.73E+04	1.26%	16.0617087	16.07221636	16.04259988	16.02756048	16.03831888	0.11%
PS(34:2)-13C	Phospholipids	7.23E+04	7.13										

Sarcosine-13C	Amino Acids and Derivatives	2.34E+06	2.04E+06	2.15E+06	2.43E+06	2.74E+06	11.59%	21.1580771	20.96013772	21.03590523	21.21252488	21.38574446	0.78%
Sedoheptulose monophosphate-13C	Sugar and Sugar Phosphate	4.35E+05	4.31E+05	4.29E+05	4.31E+05	4.33E+05	0.51%	18.72932865	18.71799765	18.70927232	18.71766304	18.72267414	0.04%
Serine-13C	Amino Acids and Derivatives	2.31E+06	2.28E+06	2.61E+06	2.25E+06	2.38E+06	6.10%	21.14195743	21.12313122	21.31782771	21.10405608	21.18495281	0.40%
Shikimic acid-13C	Organic acids	1.47E+05	1.43E+05	1.44E+05	1.53E+05	1.51E+05	2.94%	17.16250935	17.12262581	17.13270054	17.22034054	17.20131989	0.25%
Spermidine-13C	Polyamines	4.35E+06	4.39E+06	4.45E+06	4.42E+06	4.37E+06	0.89%	22.05125674	22.06447438	22.08407652	22.07430874	22.05887168	0.06%
Succinic acid-13C	Organic acids	3.53E+06	3.57E+06	3.69E+06	3.48E+06	3.51E+06	2.30%	21.75164539	21.7678967	21.81558031	21.73107038	21.74345057	0.15%
Succinyl-CoA-13C	Cofactors	6.44E+05	6.32E+05	6.04E+05	6.62E+05	6.52E+05	3.50%	19.29647712	19.26979329	19.20395015	19.33625375	19.31451244	0.26%
Sucrose-13C	Sugar and Sugar Phosphate	4.81E+07	4.83E+07	4.81E+07	4.80E+07	4.79E+07	0.36%	25.52013331	25.52611712	25.5180331	25.51502748	25.51261847	0.02%
Thiamine monophosphate-13C	Vitamins and Derivatives	2.25E+06	2.37E+06	2.35E+06	2.42E+06	2.22E+06	3.62%	21.1002106	21.17523765	21.16300098	21.20538281	21.08082793	0.25%
Thiamine-13C	Vitamins and Derivatives	1.83E+06	1.80E+06	1.93E+06	1.79E+06	1.98E+06	4.51%	20.80656221	20.77956548	20.88315636	20.77474846	20.917779745	0.31%
Threonine-13C	Amino Acids and Derivatives	5.20E+04	5.27E+04	5.32E+04	5.29E+04	5.15E+04	1.32%	15.66733334	15.68660995	15.70022295	15.69207057	15.65340492	0.12%
Thymidine-13C	Nucleosides, Nucleotides, and Analogues	4.10E+06	4.19E+06	4.32E+06	4.01E+06	3.99E+06	3.30%	21.9685993	21.99989543	22.04393509	21.93660919	21.9294029	0.22%
Thymine-13C	Nucleosides, Nucleotides, and Analogues	2.62E+06	2.75E+06	2.60E+06	2.59E+06	2.65E+06	2.44%	21.32278638	21.39257318	21.31174388	21.30619078	21.33919324	0.16%
Tryptophan-13C	Amino Acids and Derivatives	7.43E+05	7.30E+05	7.21E+05	7.27E+05	7.39E+05	1.23%	19.50377916	19.47832724	19.46003987	19.4723894	19.49599552	0.09%
Tyramine-13C	Polyamines	3.59E+04	3.50E+04	3.61E+04	3.45E+04	3.37E+04	2.84%	15.13249973	15.09589146	15.14051027	15.07514484	15.04131692	0.27%
Tyrosine-13C	Amino Acids and Derivatives	1.32E+06	1.75E+06	1.43E+06	1.61E+06	1.37E+06	11.99%	20.3321065	20.73892349	20.44758372	20.61862926	20.38574446	0.83%
UDP-13C	Nucleosides, Nucleotides, and Analogues	1.97E+06	1.83E+06	1.90E+06	2.02E+06	2.00E+06	3.91%	20.90683189	20.80577536	20.85528825	20.94306421	20.93012515	0.27%
UDP-D-glucose-13C	Nucleosides, Nucleotides, and Analogues	5.07E+05	4.87E+05	5.37E+05	5.17E+05	5.32E+05	3.90%	18.95020274	18.89208028	19.03321865	18.97840882	19.01971017	0.30%
UDP-n-acetyl-D-glucosamine-13C	Nucleosides, Nucleotides, and Analogues	7.23E+04	6.83E+04	7.03E+04	7.56E+04	7.21E+04	3.77%	16.14250598	16.06044263	16.10205771	16.20686174	16.13811178	0.34%
UMP-13C	Nucleosides, Nucleotides, and Analogues	1.39E+05	1.79E+05	1.21E+05	1.29E+05	1.30E+05	16.44%	17.08576289	17.45040581	16.88583934	16.97589274	16.98926144	1.29%
Uracil-13C	Nucleosides, Nucleotides, and Analogues	7.65E+07	7.35E+07	7.62E+07	7.55E+07	7.55E+07	1.55%	26.18857919	26.13084829	26.18290895	26.16959109	26.16959109	0.09%
Ureidosuccinic acid-13C	Amino Acids and Derivatives	2.55E+04	2.05E+04	2.10E+04	1.99E+04	2.50E+04	11.85%	14.6404709	14.32614856	14.36084708	14.28279886	14.61194694	1.17%
Uridine diphosphate glucuronic acid-13C	Nucleosides, Nucleotides, and Analogues	5.47E+05	5.41E+05	5.24E+05	5.40E+05	5.41E+05	1.59%	19.0617087	19.04580231	18.99975783	19.04126343	19.04473563	0.12%
Uridine-13C	Nucleosides, Nucleotides, and Analogues	7.67E+07	7.86E+07	7.27E+07	7.64E+07	7.58E+07	2.83%	26.19253513	26.22875999	26.11525357	26.18612482	26.17588483	0.16%
UTP-13C	Nucleosides, Nucleotides, and Analogues	3.87E+05	3.92E+05	3.67E+05	3.81E+05	3.55E+05	4.04%	18.5616012	18.58012605	18.48502738	18.53905276	18.43705305	0.32%
Valine-13C	Amino Acids and Derivatives	4.90E+07	4.95E+07	4.80E+07	4.81E+07	4.92E+07	1.46%	25.54716143	25.56179929	25.5156291	25.5180331	25.5530344	0.08%
Xanthine-13C	Nucleosides, Nucleotides, and Analogues	7.45E+04	7.41E+04	7.20E+04	7.31E+04	7.50E+04	1.63%	16.184178	16.17640693	16.13490757	16.15797845	16.19479532	0.15%
Xanthosine-13C	Nucleosides, Nucleotides, and Analogues	5.38E+04	5.32E+04	5.38E+04	5.15E+04	5.18E+04	2.09%	15.7161228	15.69778207	15.7161228	15.65290098	15.66038594	0.19%
Xanthylic acid-13C	Nucleosides, Nucleotides, and Analogues	5.74E+04	4.78E+04	5.14E+04	5.77E+04	5.14E+04	8.08%	15.80951694	15.54562817	15.64807666	15.8170336	15.65032253	0.74%

Table S4 Changes of the absolute concentrations of targeted metabolites in maize roots under Pb stress

Metabolites	Standard curve	Coefficient r	LLOD (ng/ml)	LLOQ (ng/ml)	Maize: control (µg/mg FW)	Maize: Pb treatment (µg/mg FW)	Fold change (Pb treatment/control)
1-Pyrroline-5-carboxylic acid	y=0.11915x+0.04077	0.9918	0.0132	0.058	1.248E-03±1.031E-04	1.961E-03±9.702E-04	1.57
2-Ketobutyric acid	y=0.00676x+0.027	0.9900	0.0963	0.102	0.108E-03±6.06E-05	0.0117E-03±6.05E-05	1.11
2-Keto-L-glucosamine	y=0.1914x+0.02419	0.9924	0.0145	0.017	4.912E-04±4.097E-05	5.686E-04±7.71E-05	1.16
3-hydroxy-3-methylglutaryl-CoA	y=0.008581x+0.0004061	0.9986	1.23	3.58	1.141E-03±9.522E-04	1.323692E-03±6.322E-04	1.16
3-Phosphoglyceric acid	y=0.1091x+0.2843	0.9948	2.67	6.91	11.296±0.938	11.327±0.598	1.00
4,5-Dihydroxocroic acid	y=0.08788x+0.005682	0.9921	1.05	2.91	2.522E-03±2.098E-04	1.997E-03±1.105E-04	0.79
6-Phosphogluconic acid	y=0.3373x+0.1911	0.9960	0.071	0.19	0.0186±1.562E-03	0.0164±7.651E-03	0.88
Acetic acid	y=1.321x+0.4358	0.9925	0.0081	0.013	0.326±0.0273	0.281±0.0168	0.86
Acetoacetic acid	y=0.2276x+0.003906	0.9920	0.27	0.46	0.171±0.0142	0.147±0.007382	0.86
Acetoacetyl-CoA	y=0.02979x+0.008664	0.9983	0.11	0.24	7.081E-05±5.867E-06	6.682E-05±3.881E-06	0.94
Acetylcholine	y=0.8239x+0.013517	0.9946	0.38	1.35	1.058E-03±1.04E-05	2.493E-03±2.448E-05	2.36
Acetyl-CoA	y=0.1003x+0.003014	0.9984	0.42	1.27	2.635E-03±2.194E-04	1.681E-03±8.169E-04	0.64
Acetylphosphate	y=0.8299x+1.3517	0.9956	1.82	4.91	0.155±0.0129	0.143±0.0087	0.92
Acornic acid	y=0.01074x+0.0001309	0.9965	0.54	1.13	0.533±0.0443	0.626±0.0312	1.17
Adenine	y=0.4919x+0.02243	0.9973	0.49	1.82	0.078825±0.00671	0.158±7.299E-03	2.00
Adenosine	y=1.2186x+0.06437	0.9960	0.21	0.58	0.298±0.0251	0.531±0.0342	1.78
Adenosine phosphosulfate	y=0.027816x+0.008224	0.9977	1.15	3.24	1.954E-03±1.662E-04	2.552E-03±1.786E-04	1.31
ADP	y=1.9415x+0.04689	0.9969	8.91	19.66	0.522±0.0442	0.587±0.0353	1.13
ADP-glucose	y=0.02983x+0.006044	0.9959	0.69	1.23	5.688E-03±7.646E-04	4.903E-03±2.345E-04	0.86
Agmatine	y=0.01197x+0.0173	0.9925	1.08	8.45	0.146±0.0121	0.302±0.0168	2.07
Alanine	y=1.4576x+2.6284	0.9920	4.79	11.63	1.115±0.0926	1.824±0.0983	1.64
Alpha-ketoglutaric acid	y=0.003062x+0.1783	0.9994	0.17	0.44	0.0568±4.731E-03	0.0784±4.171E-03	1.38
Aminoadipic acid	y=0.007927x+0.02475	0.9992	1.95	3.01	9.574E-05±7.983E-06	1.457E-05±7.016E-06	0.15
AMP	y=1.15305x+0.1283	0.9947	0.085	0.33	0.558±0.0464	0.352±0.0174	0.63
Arginine	y=1.2371x+0.1351	0.9998	0.11	0.43	0.348±0.0292	0.544±0.0341	1.56
Ascorbic acid	y=0.04547x+0.004403	0.9986	0.37	1.82	2.251±0.187	3.719±0.179	1.65
Asparagine	y=3.251x+0.1256	0.9905	0.065	0.109	1.697±0.141	2.067±0.122	1.21
Aspartic acid	y=1.3856x+0.0676	0.9993	1.79	4.64	5.103±0.432	6.235±0.314	1.23
ATP	y=0.1824x+1.456	0.9979	4.78	10.62	1.692±0.141	1.045±0.0583	0.62
Benzoic acid	y=1.225x+0.01564	0.9985	0.19	0.35	0.821±0.0686	0.835±0.03945	1.02
Beta-alanine	y=0.06628x+0.0018254	0.9917	0.69	1.42	37.323±3.118	34.165±2.045	1.29
Carbamoyl-phosphate	y=0.0273x+0.4153	0.9963	0.43	0.79	0.166±0.0138	0.211±0.0106	1.27
CDP	y=0.09642x+0.001028	0.9939	0.27	0.63	0.416±0.0346	0.282±0.0152	0.68
Choline	y=2.6713x+0.000013	0.9949	4.85	12.23	1.306±0.175	1.401±0.0979	1.07
Citric acid	y=15.91x+0.005028	0.9992	0.0065	0.0091	36.112±0.017	45.402±0.721	1.26
Citulline	y=0.8699x+0.00649	0.9911	0.41	1.21	0.137±0.0259	0.1702±0.286	1.24
CMP	y=5.5249x+0.04093	0.9958	0.89	1.15	0.0311±2.905E-03	0.0344±1.653E-03	1.11
Coenzyme A	y=0.0363x+0.0285	0.9989	0.56	3.01	1.274E-03±1.062E-04	1.202E-03±5.801E-04	0.94
CTP	y=0.1355x+0.01681	0.9938	0.14	0.46	0.808±0.0691	0.711±0.0512	0.88
cyclic AMP	y=0.1298x+0.00166	0.9964	0.091	0.23	1.061E-04±8.895E-05	4.148E-05±2.583E-06	0.39
Cystathionine	y=0.01106x+0.002461	0.9893	0.72	2.15	0.0208±1.721E-03	0.0156±7.785E-03	0.75
Cysteine	y=0.779x+0.01128	0.9930	0.11	0.43	0.2317±0.0195	0.417±0.0193	1.80
Cytidine	y=0.1958x+0.014141	0.9972	0.24	0.79	0.179±0.0149	0.242±0.0134	1.35
Cytosine	y=0.2437x+0.02316	0.9902	1.08	3.45	0.144±0.0121	0.133±0.0784	0.92
dADP	y=0.0396x+0.0008992	0.9977	1.81	2.53	1.168E-03±7.930E-04	1.013E-03±6.416E-04	0.87
dAMP	y=0.06229x+0.0022915	0.9958	0.19	0.99	1.256E-03±7.343E-04	1.123E-03±9.391E-04	0.92
dATP	y=0.3964x+0.05313	0.9933	0.41	1.52	2.41E-03±2.007E-04	2.292E-03±1.147E-04	0.95
dCDP	y=3.4710x+0.001974	0.9969	0.26	0.51	3.414E-04±2.839E-05	4.4582E-04±2.225E-05	1.31
dCMP	y=5.5638x+0.02259	0.9958	0.14	0.81	5.211E-04±4.378E-05	5.554E-04±2.579E-05	1.07
dCTP	y=0.01264x+0.0002379	0.9947	0.52	1.14	9.684E-04±8.047E-05	4.167E-04±6.209E-05	0.43
Deoxyadenosine	y=0.06214x+0.000462	0.9979	0.46	0.62	5.199E-04±4.337E-05	6.251E-04±3.016E-05	1.20
Deoxyguanosine	y=0.00137x+0.00001131	0.9969	0.79	1.91	6.931E-04±5.795E-05	6.586E-04±3.115E-05	NA
Deoxyinosine	y=0.0111x+0.00000928	0.9966	0.46	1.57	9.031E-05±5.880E-06	9.838E-05±5.880E-06	NA
Deoxyribose phosphate	y=0.04743x+0.005992	0.9981	0.092	0.29	5.711E-04±4.771E-05	5.534E-04±2.717E-05	NA
Deoxyuridine	y=0.4986x+0.0002788	0.9977	0.33	1.01	1.444E-04±1.201E-05	1.656E-04±9.121E-06	NA
Dephospho-CoA	y=0.0011x+0.01236	0.9984	0.097	0.29	1.201E-05±1.024E-06	8.372E-06±4.706E-06	NA
dGDP	y=0.1281x+0.01103	0.9946	0.52	1.21	2.643E-04±2.197E-05	3.012E-04±1.518E-05	NA
dGMP	y=0.001405x+0.001244	0.9946	0.48	1.19	2.511E-04±2.087E-05	2.829E-04±1.444E-05	NA
dGTP	y=0.2215x+0.039158	0.9931	0.36	0.99	3.873E-03±1.226E-04	3.628E-03±1.768E-04	NA
dIMP	y=0.24152x+0.003952	0.9935	0.12	0.27	3.572E-05±2.968E-06	2.912E-05±1.514E-06	NA
dITP	y=0.1543x+0.3808	0.9945	0.08	0.16	9.795E-05±4.181E-06	1.1254E-04±5.876E-05	NA
dUTP	y=0.19699x+0.007916	0.9935	0.39	0.58	1.148E-04±3.487E-04	9.867E-04±4.891E-05	NA
dUDP-D-glucose	y=0.03643x+2.435	0.9852	0.71	1.38	0.133±0.011	0.0968±0.00488	0.73
dTMP	y=0.1824x+0.02131	0.9965	0.15	0.37	5.786E-04±4.815E-05	5.825E-04±3.257E-05	1.01
dTTP	y=0.1243x+0.03466	0.9937	0.23	0.64	9.590E-05±7.968E-05	4.101E-05±3.704E-06	0.43
dUMP	y=0.07424x+0.0009294	0.9945	0.38	1.23	2.642E-05±2.362E-06	1.952E-05±2.561E-06	0.74
dUTP	y=0.02386x+0.01722	0.9944	0.47	1.92	9.720E-04±8.079E-05	5.172E-04±6.345E-05	0.53
Erythrose 4-phosphate	y=0.002178x+0.05006	0.9914	0.055	0.165	0.0128±1.071E-04	0.0124±6.211E-04	0.97
Ethanolamine	y=0.01384x+0.0099406	0.9926	1.31	3.25	0.0453±3.755E-03	0.0231±1.147E-03	0.51
FAD	y=0.14427x+0.0040854	0.9937	0.48	1.55	3.445E-02±1.363E-03	2.331E-02±1.188E-03	0.68
Farnesyl diphosphate	y=0.5014x+0.09443	0.9982	0.54	1.32	0.246±0.0205	0.345±0.01741	1.40
FMN	y=0.04681x+0.005011	0.9982	1.89	2.91	5.322E-03±4.422E-04	3.223E-03±1.657E-04	0.61
Fumaric acid	y=0.5856x+0.01608	0.9995	0.15	0.24	0.0844±7.021E-03	0.1435±7.023E-03	1.69
Gamma-Aminobutyric acid	y=0.009372x+0.004264	0.9985	2.64	7.18	1.724±0.143	3.781±0.143	1.61
GDP	y=0.2184x+0.07534	0.9936	0.35	1.42	1.006E-04±8.367E-05	1.347E-04±8.621E-05	1.34
Geranyl-PP	y=0.1258x+0.018293	0.9939	0.11	0.29	2.07E-04±1.732E-05	1.846E-04±8.975E-05	0.89
Glucaric acid	y=0.16177x+0.005384	0.9963	0.28	0.64	2.511E-04±2.088E-05	2.054E-04±1.125E-05	0.82
Glucic acid	y=0.1618x+0.0005384	0.9906	0.015	0.049	0.0561±4.671E-03	0.1002±5.051E-03	1.79
Glucosamine	y=0.22x+0.04310	0.9812	0.57	1.24	2.475E-05±2.049E-06	3.293E-05±1.801E-06	1.33
Glucosamine 6-phosphate	y=0.00771x+0.0002029	0.9836	0.078	0.23	3.081E-04±2.564E-05	2.239E-04±1.251E-05	0.73
Glutamic acid	y=0.02816x+0.00984	0.9913	0.57	1.71	0.0291±2.421E-03	0.0384±1.965E-03	1.32
Glutamine	y=0.4986x+0.05347	0.9991	0.089	0.153	4.103±0.342	7.709±0.371	1.88
Glutamine	y=1.622x+0.025903	0.9911	0.14	0.45	1.361±0.114	1.667±0.0788	1.22
Glyceralddehyde	y=0.223x+0.0002	0.9948	2.48	7.44	1.496±0.395	1.456±0.292	0.87
Glyceralddehyde 3-phosphate	y=0.7085x+0.003266	0.9951	3.58	11.52	0.145±0.0121	0.1527±3.53E-03	1.05
Glyceric acid	y=0.3263x+0.0002038	0.9911	1.69	6.78	0.0191±1.591E-03	0.0264±1.291E-03	1.38
Glycerol	y=0.9193x+0.027	0.9953	8.13	24.21	0.269±0.0228	0.307±0.0208	1.14
Glycerol 3-phosphate	y=0.7995x+0.01122	0.9941	0.54	1.25	0.0691±5.750E-03	0.0631±3.548E-03	0.91
Glycerophosphocholine	y=0.2562x+0.0007	0.9950	10.18	21.64	0.102±0.00855	0.0636±0.00304	0.62
Glycine	y=0.1077x+0.0376	0.9911	4.56	15.91	0.289±0.0241	0.224±0.0134	0.78
Glycolic acid	y=1.1258x+0.02747	0.9913	0.42	1.67	0.0614±5.12E-03	0.0601±3.12E-03	0.98
Glyoxylac acid	y=0.8103x+0.01615	0.9925	1.78	4.21	0.0396±3.291E-03	0.0374±1.957E-03	0.94
GMP	y=0.2415x+0.01674	0.9935	0.39	1.11	2.391E-03±1.988E-04	2.016E-03±1.013E-04	0.84
GTP	y=0.2373x+0.003156	0.9930	0.98	0.41	0.027815±2.314E-03	0.03221±1.801E-03	1.16
Guanine	y=0.1883x+0.00004256	0.9971	0.13	0.55	7.251E-03±6.028E-04	5.599E-03±3.036E-04	0.77
Guanosine	y=0.01731x+0.008915	0.9968	0.59	1.32	0.132±0.0109	0.114±0.00641	0.87
Hexose biphosphate	y=1.165x+0.3801	0.9997	1.59	4.91	0.725±0.0612	0.471±0.0284	0.64
Hexose monophosphate	y=0.897x+0.1308	0.9998	1.62	3.68	0.119±9.905E-03	0.175±9.928E-03	1.47
Hexose pool	y=9.936x+0.006423	0.9996	5.11	13.47	57.661±4.791	49.105±2.577	0.85
Histidine	y=0.1722x+0.03391	0.9997	0.19	0.27	0.268±0.0223	0.453±0.0249	1.69
Homocysteine	y=0.1645x+0.01356	0.9918	0.39	1.43	1.45E-03±1.207E-04	1.454471E-03±7.331E-04	1.00
Homoserine	y=0.01679x+0.007204	0.9900	4.75	15.98	0.4651±0.03865	0.417±0.0212	0.90
Hydroxyphenyllactic acid	y=0.01763x+0.02162	0.9914	16.91	30.28	0.0141±1.162E-03	0.0131±6.621E-03	0.93
Hypoxanthine	y=0.4283x+0.003355	0.9967	1.45	3.252	0.0483±3.182E-03	0.0712±4.003E-03	1.47
IMP	y=0.1543x+0.3808	0.9950	0.191	0.311	2.539E-05±2.11E-04	3.071E-05±1.612E-04	1.21
IMP	y=0.09815x+0.01637	0.9914	0.27	0.84	0.0990±7.231E-03	0.1086±4.141E-03	1.20
Inosine	y=0.43711x+0.0						

NADPH	y=0.135x+0.0307	0.9944	0.052	0.19	0.0364+3.046E-03	0.0501+2.595E-03	1.38
Niacinamide	y=0.659x+0.005206	0.9896	0.071	0.292	7.94576E-04+6.621E-05	8.895E-04+4.323E-05	1.12
Nicotinic acid	y=0.194x+0.0112	0.9973	0.048	0.144	6.254E-04+5.214E-05	7.354E-04+5.541E-05	1.17
Oleic acid	y=0.022x+0.000432	0.9938	1.91	4.88	4.709E-04+4.006E-05	6.347E-04+4.441E-05	1.35
Oxalimide	y=0.579x+0.0902	0.9995	2.17	6.05	0.116x+0.644E-03	0.089x+0.439E-03	0.77
Orothidic acid	y=1.501E-03x+0.239	0.9942	0.91	2.15	2.184E-03+1.815E-04	1.983E-03+1.009E-04	0.91
Oxalic acid	y=1.8201x+0.0183	0.9975	0.38	1.08	1.488x+0.124	1.432+0.0731	0.96
Oxaloacetic acid	y=0.0367x+0.00243	0.9904	0.14	0.58	2.386E-03+1.986E-04	2.184E-03+1.073E-04	0.92
Oxidized glutathione	y=0.4711x+0.001121	0.9990	0.78	2.15	0.0226+1.883E-03	0.01208+6.542E-03	0.53
Oxoglutaric acid	y=1.563x+0.03231	0.9971	0.58	1.91	0.278+0.0231	0.2079+0.0104	0.75
PA(28.0)	y=0.05721x+0.001685	0.9923	2.18	5.47	ND	ND	ND
PA(28.1)	y=0.05721x+0.001685	0.9923	2.18	5.47	ND	ND	ND
PA(30.0)	y=0.05438x+0.001579	0.9910	2.18	5.47	ND	ND	ND
PA(30.1)	y=0.05438x+0.001579	0.9909	2.18	5.47	ND	ND	ND
PA(32.0)	y=0.05438x+0.001580	0.9903	2.18	5.47	ND	ND	ND
PA(32.1)	y=0.05438x+0.001581	0.9902	2.18	5.47	5.919E-05+4.914E-06	8.066E-05+4.337E-06	1.36
PA(32.2)	y=0.05438x+0.001581	0.9997	2.18	5.47	ND	ND	ND
PA(34.1)	y=0.05279x+0.002581	0.9997	2.31	5.55	0.0313+2.682E-03	0.0563+4.052E-03	1.80
PA(34.2)	y=0.05279x+0.002581	0.9997	2.31	5.55	0.03725+3.123E-03	0.07512+4.689E-03	2.02
PA(34.3)	y=0.05279x+0.002582	0.9997	2.31	5.55	0.0516+4.295E-03	0.113+6.251E-03	2.19
PA(36.1)	y=0.05279x+0.002581	0.9931	2.31	5.55	ND	ND	ND
PA(36.2)	y=0.05279x+0.002581	0.9994	2.31	5.55	0.0194+1.651E-03	0.0547+3.723E-03	2.82
PA(36.4)	y=0.05279x+0.002582	0.9997	2.31	5.55	0.0488+2.412E-03	0.121+7.26E-02	2.48
PA(36.5)	y=0.05279x+0.002583	0.9997	2.31	5.55	0.0446+2.052E-03	0.113+5.62E-02	2.53
PA(36.6)	y=0.05279x+0.002584	0.9997	2.31	5.55	0.0378+1.648E-03	0.0991+4.042E-03	2.64
p-Aminobenzoic acid	y=0.1357x+0.007926	0.9906	0.58	1.43	8.126E-03+6.757E-04	7.082E-03+3.959E-04	0.87
Pantoic acid	y=0.1371x+0.03129	0.9900	0.079	0.25	2.912E-02+4.242E-04	5.602E-03+3.154E-04	1.92
PC(22.0)	y=0.2860x+0.002759	0.9923	1.94	5.16	ND	ND	ND
PC(22.1)	y=0.2860x+0.002759	0.9921	1.94	5.16	ND	ND	ND
PC(24.0)	y=0.2860x+0.002759	0.9920	1.94	5.16	ND	ND	ND
PC(24.1)	y=0.2860x+0.002759	0.9918	1.94	5.16	ND	ND	ND
PC(26.0)	y=0.2860x+0.002759	0.9996	1.94	5.16	ND	ND	ND
PC(26.1)	y=0.2860x+0.002759	0.9913	1.94	5.16	ND	ND	ND
PC(28.0)	y=0.2860x+0.002759	0.9908	1.94	5.16	ND	ND	ND
PC(28.1)	y=0.2860x+0.002759	0.9900	1.94	5.16	ND	ND	ND
PC(28.2)	y=0.2860x+0.002759	0.9992	1.94	5.16	ND	ND	ND
PC(30.0)	y=0.2670x+0.006771	0.9986	1.85	5.01	ND	ND	ND
PC(30.1)	y=0.2670x+0.006771	0.9901	1.85	5.01	ND	ND	ND
PC(30.2)	y=0.2670x+0.006771	0.9984	1.85	5.01	ND	ND	ND
PC(32.0)	y=0.2670x+0.006771	0.9984	1.85	5.01	ND	ND	ND
PC(32.1)	y=0.2670x+0.006771	0.9981	1.85	5.01	ND	ND	ND
PC(32.2)	y=0.2670x+0.006771	0.9978	1.85	5.01	ND	ND	ND
PC(34.1)	y=0.2983x+0.005961	0.9976	1.79	4.95	2.161+0.179	1.974+0.106	0.91
PC(34.2)	y=0.2983x+0.005961	0.9976	1.79	4.95	1.947+0.162	1.824+0.0987	0.93
PC(34.3)	y=0.2983x+0.005961	0.9976	1.79	4.95	3.477+0.289	3.928+0.201	1.13
PC(36.0)	y=0.2983x+0.005961	0.9976	1.79	4.95	ND	ND	ND
PC(36.1)	y=0.2983x+0.005961	0.9972	1.79	4.95	0.575+0.0479	0.549+0.0276	0.95
PC(36.2)	y=0.2983x+0.005961	0.9976	1.79	4.95	1.301+0.108	1.062+0.0594	0.82
PC(36.3)	y=0.2983x+0.005961	0.9976	1.79	4.95	1.943+0.162	1.7367+0.0948	0.89
PC(36.4)	y=0.2983x+0.005961	0.9974	1.79	4.95	3.094+0.257	2.752+0.257	0.92
PC(36.5)	y=0.2983x+0.005961	0.9974	1.79	4.95	2.941+0.245	2.183+0.122	0.74
PC(36.6)	y=0.2983x+0.005961	0.9974	1.79	4.95	2.707+0.225	1.418+0.0744	0.52
PC(38.3)	y=0.2983x+0.005961	0.9974	1.79	4.95	0.0749+6.251E-03	0.102+0.067E-03	1.36
PC(38.5)	y=0.2983x+0.005961	0.9974	1.79	4.95	0.0515+4.291E-03	0.0477+2.352E-03	0.93
PE(28.0)	y=0.3693x+0.007644	0.9955	4.32	11.56	ND	ND	ND
PE(28.1)	y=0.3693x+0.007644	0.9952	4.32	11.56	ND	ND	ND
PE(30.0)	y=0.3693x+0.007644	0.9955	4.32	11.56	ND	ND	ND
PE(30.1)	y=0.3693x+0.007644	0.9955	4.32	11.56	ND	ND	ND
PE(30.2)	y=0.3693x+0.007644	0.9955	4.32	11.56	ND	ND	ND
PE(32.1)	y=0.3712x+0.008691	0.9955	4.17	11.38	ND	ND	ND
PE(32.2)	y=0.3712x+0.008691	0.9955	4.17	11.38	ND	ND	ND
PE(34.1)	y=0.3712x+0.008691	0.9955	4.17	11.38	0.293+0.0244	0.256+0.0125	0.87
PE(34.2)	y=0.3712x+0.008691	0.9955	4.17	11.38	0.985+0.0819	0.711+0.0399	0.72
PE(34.3)	y=0.3712x+0.008691	0.9955	4.17	11.38	1.171+0.0973	0.707+0.0356	0.60
PE(36.1)	y=0.3712x+0.008691	0.9957	4.17	11.38	0.0884+7.351E-03	0.0499+2.565E-03	0.56
PE(36.2)	y=0.3712x+0.008691	0.9957	4.17	11.38	0.155+0.0129	0.134+6.551E-03	0.86
PE(36.3)	y=0.3712x+0.008691	0.9957	4.17	11.38	0.674+0.0561	0.551+0.0271	0.82
PE(36.4)	y=0.3712x+0.008691	0.9957	4.17	11.38	1.161+0.0992	0.712+0.0329	0.61
PG(22.0)	y=0.6508x+0.04281	0.9937	5.82	9.63	0.843+0.0718	0.663+0.0305	0.78
PG(42.1)	y=0.6508x+0.04281	0.9937	5.82	9.63	0.435+0.0371	0.241+0.0167	0.55
PG(42.2)	y=0.6508x+0.04281	0.9937	5.82	9.63	ND	ND	ND
PG(44.1)	y=0.6508x+0.04281	0.9937	5.82	9.63	1.249+0.105	0.578+0.0391	0.46
PG(44.2)	y=0.6508x+0.04281	0.9937	5.82	9.63	0.948+0.0791	0.743+0.0355	0.78
Phenylalanine	y=1.793x+0.02122	0.9932	1.97	4.66	2.258+0.187	1.997+0.101	0.88
Phenylacetic acid	y=0.05875x+0.05397	0.9923	0.14	0.32	0.0308+2.561E-03	0.0236+1.293E-03	0.77
Phenylpyruvic acid	y=0.0589x+0.3377	0.9922	0.28	0.53	1.123E-04+9.348E-05	9.901E-05+5.532E-05	0.88
Phosphoenolpyruvic acid	y=0.6588x+0.001023	0.9944	1.14	4.21	0.0761+6.351E-03	0.0689+3.471E-03	0.91
Phosphoenolpyruvate	y=0.6484x+0.00531	0.9945	1.14	4.21	0.254+0.012	0.243+0.0124	0.95
Phosphorylcholine	y=0.5219x+0.000007	0.9939	0.63	1.45	0.145+0.0121	0.161+0.0599	1.11
Phosphoserine	y=2.576x+0.001351	0.9960	0.72	2.11	0.0291+2.424E-03	0.0327+1.594E-03	1.12
PI(26.0)	y=0.1571x+0.03128	0.9944	1.03	3.29	ND	ND	ND
PI(28.0)	y=0.1571x+0.03128	0.9944	1.03	3.29	ND	ND	ND
PI(28.1)	y=0.1571x+0.03128	0.9944	1.03	3.29	ND	ND	ND
PI(30.0)	y=0.1571x+0.03128	0.9944	1.03	3.29	ND	ND	ND
PI(30.1)	y=0.1571x+0.03128	0.9944	1.03	3.29	ND	ND	ND
PI(30.2)	y=0.1571x+0.03128	0.9944	1.03	3.29	ND	ND	ND
PI(32.0)	y=0.1639x+0.04372	0.9985	0.93	3.05	ND	ND	ND
PI(32.1)	y=0.1639x+0.04372	0.9944	0.93	3.05	ND	ND	ND
PI(32.2)	y=0.1639x+0.04372	0.9944	0.93	3.05	ND	ND	ND
PI(34.0)	y=0.1639x+0.04372	0.9985	0.93	3.05	ND	ND	ND
PI(34.1)	y=0.1639x+0.04372	0.9970	0.93	3.05	1.608+0.133	1.356+0.0678	0.84
PI(34.2)	y=0.1639x+0.04372	0.9955	0.93	3.05	3.421+0.284	4.455+0.2223	1.30
PI(34.3)	y=0.1639x+0.04372	0.9955	0.93	3.05	5.115+0.429	7.459+0.3463	1.46
PI(36.1)	y=0.1605x+0.06348	0.9980	0.91	3.42	0.0253+2.103E-03	0.0232+1.235E-03	0.92
PI(36.2)	y=0.1605x+0.06348	0.9954	0.91	3.42	0.0361+3.005E-03	0.0319+1.335E-03	0.88
Prophosphate	y=0.01172x+0.1357	0.9999	0.13	0.29	1.549E-05+1.291E-06	1.366E-05+7.755E-06	0.88
Proline	y=0.3250x+0.1680	0.9922	0.25	0.44	0.943+0.0785	1.531+0.0752	1.62
Propionyl-CoA	y=0.09152x+0.007086	0.9988	1.21	2.84	3.828E-04+3.186E-05	5.341E-04+2.631E-05	1.40
PS(32.0)	y=0.07136x+0.0002398	0.9972	3.01	6.55	ND	ND	ND
PS(32.1)	y=0.07136x+0.0002398	0.9971	3.01	6.55	ND	ND	ND
PS(32.2)	y=0.07136x+0.0002398	0.9965	3.01	6.55	ND	ND	ND
PS(34.1)	y=0.0662x+0.0001517	0.9948	2.87	6.38	0.0277+2.308E-03	0.0153+7.693E-03	0.55
PS(34.2)	y=0.0662x+0.0001517	0.9947	2.87	6.38	0.0249+2.072E-03	0.0131+6.669E-04	0.53
PS(34.3)	y=0.0662x+0.0001517	0.9947	2.87	6.38	0.0351+2.925E-03	0.0274+1.531E-03	0.78
PS(36.0)	y=0.0683x+0.0002432	0.9940	2.81	6.09	ND	ND	ND
PS(36.2)	y=0.0683x+0.0002432	0.9934	2.81	6.09	0.0539+4.483E-03	0.0475+0.002.481E-03	0.88
Putrescine	y=0.1845x+0.0002848	0.9901	3.55	6.27	0.0487+4.058E-03	0.0673+3.3871E-03	1.38
Pyridoxine	y=0.011653x+0.001856	0.9922	0.25	0.62	3.401E-05+2.814E-06	3.006E-05+1.516E-06	0.88
Pyroglutamic acid	y=0.01398x+0.002955	0.9915	0.079	0.23	3.38E-03+6.975E-04	0.0108+5.471E-04	1.29
Pyruvic acid	y=2.072x+0.031	0.9914	0.44	1.32	0.7961+0.0615	0.5925+0.03109	0.74
Quinolinic acid	y=5.535x+0.005942	0.9965	0.12	0.28	1.171E-03+9.774E-04	2.286E-03+3.665E-04	1.95
Reduced glutathione	y=0.3421x+0.001038	0.9901	0.37	1.35	0.1127E-03+3.81E-05	0.295+0.0465	2.62
Riboflavin	y=0.08462x+0.0001534	0.9901	0.27	0.51	4.478E-04+3.721E-05	6.496E-04+3.341E-05	1.45
Ribose 5-phosphate	y=0.1719x+0.07857	0.9970	1.12	1.12	5.281E-02+4.396E-03	6.391E-02+3.231E-03	1.21
S-Adenosylhomocysteine	y=0.4296x+0.03393	0.9995	0.24	0.63	7.06442E-04+5.859E-05	1.296E-03+7.083E-05	1.83
S-Adenosylmethionine	y=1.735x+0.01368	0.9906	0.18	0.29	2.655E-03+2.209E-04	3.301E-03+1.849E-04	1.24
Sarcosine	y=1.539x+0.00024	0.9920	1.23	3.87	0.131+0.0108	0.175+0.00983	1.34
Sedoheptulose monophosphate	y=0.005701x+0.0001022	0.9912	0.11	0.36	1.061E-04+8.864E-05	1.435E-04+7.865E-05	1.35
Serine	y=0.1832x+2.279	0.9999	1.99	4.23	0.725+0.0603	0.963+0.0595	

Thymine	$y=0.201x+0.000027$	0.9982	0.21	0.33	$1.154E-03+9.628E-04$	$8.814E-04+4.254E-05$	0.76
Tryptophan	$y=0.6175x+0.006685$	0.9930	0.83	3.32	$0.283+0.0235$	$0.601+0.0303$	2.12
Tyramine	$y=0.1391x+0.02876$	0.9909	1.56	3.09	$5.799E-04+4.819E-05$	$7.001E-04+5.622E-05$	1.21
Tyrosine	$y=0.0013x+0.0000029$	0.9920	2.68	5.77	$2.239+0.194$	$2.223+0.121$	0.95
UDP	$y=0.01679x+0.007204$	0.9934	0.91	2.73	$2.664E-03+2.218E-04$	$3.264E-03+1.837E-04$	1.23
UDP-D-glucose	$y=0.2503x+0.008295$	0.9957	0.19	0.51	$0.128+0.0107$	$0.113+5.708E-03$	0.88
UDP-n-acetyl-D-glucosamine	$y=0.1883x+0.00004256$	0.9856	0.23	0.64	$2.215E-05+1.838E-06$	$1.797E-05+9.138E-06$	0.81
UMP	$y=0.7886x+0.01429$	0.9955	1.63	4.14	$0.0152+1.273E-03$	$0.0147+7.201E-03$	0.97
Uracil	$y=0.1051x+0.0001018$	0.9981	3.91	11.45	$0.157+0.0131$	$0.303+0.0149$	1.93
Ureidoucetic acid	$y=0.03015x+0.006332$	0.9906	0.33	0.95	$0.0243+2.023E-03$	$0.0287+1.511E-03$	1.18
Uridine	$y=0.4504x+0.0004251$	0.9939	2.43	7.91	$0.109+0.00931$	$0.295+0.01365$	2.71
Uridine diphosphate glucuronic acid	$y=0.05135x+0.008737$	0.9975	0.71	3.15	$3.695E-05+3.169E-06$	$5.148E-05+2.396E-06$	1.39
UTP	$y=2.6053x+0.0093252$	0.9948	0.77	2.65	$0.337+0.0287$	$0.327+0.0238$	0.97
Valine	$y=9.8124x+0.0006$	0.9929	1.98	3.52	$1.494+0.125$	$2.187+0.102$	1.46
Xanthine	$y=0.1757x+0.003759$	0.9963	0.17	0.37	$0.0503+4.231E-03$	$0.0412+2.651E-03$	0.82
Xanthosine	$y=0.31658x+0.07428$	0.9961	0.31	0.74	$3.578E-04+3.02915E-05$	$3.631E-04+2.457E-05$	1.01
Xanthylic acid	$y=0.1438x+0.0002855$	0.9962	0.47	0.93	$2.486E-05+2.08169E-06$	$2.185E-05+1.035E-06$	0.88

Table S5 The abbreviation of the metabolites listed on pathway map

Compound	Abbreviation	Pathway
6-Phosphogluconic acid	6PGC	Pentose-phosphate pathway
6-Phosphonoglucono-D-lactone	6PGL	Pentose-phosphate pathway
Acetylcholine	Acho	Glycerolipid metabolism
Acetyl-CoA	ACCOA	Glycolysis
Aconitic acid	ACONT	TCA cycle
Adenine	Ade	Purine metabolism
Adenosine	ADO	Purine metabolism
ADP-Glucose	ADPGlu	Starch biosynthesis
CDP-choline	CDP-Cho	Glycerolipid metabolism
CDP-ethanolamine	CDP-ETA	Glycerolipid metabolism
Choline	Cho	Glycerolipid metabolism
Citric acid	CIT	TCA cycle
Cytidine	CTD	Pyrimidine metabolism
Cytosine	CTO	Pyrimidine metabolism
Deoxyadenosine	Dado	Purine metabolism
Deoxycytidine	Dctd	Pyrimidine metabolism
Deoxyguanosine	dGAO	Purine metabolism
Deoxyinosine	Dino	Purine metabolism
Deoxyuridine	Durd	Pyrimidine metabolism
Erythrose 4-phosphate	E4P	Pentose-phosphate pathway
Ethanolamine	ETA	Glycerolipid metabolism
Fructose 1,6-bisphosphate	F1,6P	Glycolysis
Fructose 6-phosphate	F6P	Pentose-phosphate pathway
Fumaric acid	FUM	TCA cycle
Gluconic acid	Gluc	Pentose-phosphate pathway
Glucose	Glu	Glycolysis
Glucose-1-phosphate	G1P	Glycolysis
Glucose-6-phosphate	G6P	Glycolysis
Glyceraldehyde	GAD	Glycerolipid metabolism
Glyceraldehyde 3-phosphate	GA3P	Glycolysis
Glycerate-2-phosphate	GA2P	Glycolysis
Glyceric acid	GA	Glycerolipid metabolism
Glycerol	GLO	Glycerolipid metabolism
Guanine	GAN	Purine metabolism
Guanosine	GAO	Purine metabolism
Hypoxanthine	HPX	Purine metabolism
Inosine	INO	Purine metabolism
Isocitrate	ISOCIT	TCA cycle
Lysophosphatidic acid	LPA	Glycerolipid metabolism
Malic acid	MAL	TCA cycle
Myoinositol	Ins	Glycerolipid metabolism
Orotidylic acid	OMP	Pyrimidine metabolism
Oxaloacetic acid	OAA	TCA cycle
Oxoglutaric acid	2-OGA	TCA cycle
Phosphatidic acid	PA	Glycerolipid metabolism
Phosphatidylcholine	PC	Glycerolipid metabolism
Phosphatidylglycerol	PG	Glycerolipid metabolism
Phosphatidylinositol	PI	Glycerolipid metabolism
Phosphatidylserine	PS	Glycerolipid metabolism
Phosphoenolpyruvic acid	PEP	Glycolysis
Phosphoribosyl pyrophosphate	PRPP	Pentose-phosphate pathway
Phosphorylcholine	PCH	Glycerolipid metabolism
Phosphorylethanolamine	PETA	Glycerolipid metabolism
Pyruvic acid	PYR	Glycolysis
Ribose 5-phosphate	R5P	Pentose-phosphate pathway
Ribulose 5-phosphate	Ru5P	Pentose-phosphate pathway
Sedoheptulose 7-phosphate	S7P	Pentose-phosphate pathway
Serine	Ser	Glycerolipid metabolism
Starch	Starch	Starch biosynthesis
Succinic acid	SUC	TCA cycle
Succinyl-CoA	SUCCOA	TCA cycle

Sucrose	SUC	Photosynthesis
TDP-Glucose	TDPGlu	Pyrimidine metabolism
Thymidine	THD	Pyrimidine metabolism
Thymine	THM	Pyrimidine metabolism
UDP-Glucose	UDPGlu	Glycerolipid metabolism
Uracil	URA	Pyrimidine metabolism
Uridine	URD	Pyrimidine metabolism
xanthine	XAN	Purine metabolism
Xanthosine	XAO	Purine metabolism
Xanthosine 5-phosphate	XMP	Purine metabolism
Xylulose-5-phosphate	X5P	Pentose-phosphate pathway