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=0.006705x+0.02787	0.9900	0.0963	0.102	0.0105±8.702E-03	0.0117±6.305E-03	1.11
2-Keto-L-gluconate	y=0.1914x+0.02419	0.9924	0.0145	0.037	4.912E-04±4.097E-05	5.686E-04±2.737E-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-Dihydroorotic 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±3.3881E-06	0.94
Acetylcholine	y=0.8299x-0.013517	0.9946	0.38	1.35	1.058E-02±1.104E-03	2.492E-02±3.448E-03	2.36
Acetyl-CoA	y=0.1003x+0.003014	0.9984	0.42	1.27	2.633E-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±0.0687	0.92
Aconitic 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	0.5875±0.0353	1.13
ADP-glucose	y=0.02983x+0.006044	0.9959	0.69	1.23	5.686E-03±4.746E-04	4.902E-03±2.345E-04	0.86
Agmatine	y=0.03197x+0.0173	0.9925	3.08	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-ketoisovaleric 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+0.1551	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-0.1236	0.9905	0.065	0.109	1.697±0.141	2.061±0.122	1.21
Aspartic acid	y=1.2856x-0.0676	0.9993	1.79	6.64	5.103±0.432	6.235±0.314	1.22
ATP	y=0.1824x+1.456	0.9979	4.78	10.62	1.692±0.141	1.0445±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=0.06682x+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=2.671x+0.000013	0.9949	4.85	12.23	1.306±0.175	1.401±0.0979	1.07
Citric acid	y=15.91x+0.0005028	0.9992	0.0065	0.0091	36.112±3.017	45.402±2.721	1.26
Citrulline	y=0.8699x+0.08649	0.9911	0.44	1.21	18.394±1.529	13.702±2.856	0.74
CMP	y=0.5249x+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	1.56	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±2.5835E-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+0.00006992	0.9977	0.23	1.04	1.168E-03±7.939E-04	1.012E-03±8.614E-04	0.87
dAMP	y=0.06229x+0.0022915	0.9958	0.19	0.99	1.226E-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=0.56388x+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=0.001337x+0.0000111131	0.9969	0.79	1.91	6.931E-04±5.795E-05	6.586E-04±3.115E-05	NA
Deoxyinosine	y=0.011161x+0.000006928	0.9966	0.66	1.57	9.031E-05±7.534E-06	9.838E-05±5.886E-06	NA
Deoxyribose phosphate	y=0.04743x+0.005992	0.9981	0.092	0.29	5.731E-04±4.771E-05	5.534E-04±2.718E-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±3.2263-04	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±8.141E-06	1.1254E-04±5.876E-05	NA
dTDP	y=0.19609x+0.007916	0.9953	0.19	0.54	1.140E-03±9.487E-04	9.867E-04±4.891E-05	0.87
dTDP-D-Glucose	y=0.03643x+2.435	0.9852	0.71	1.38	0.133±0.0111	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±3.7004E-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+0.0009406	0.9926	1.31	3.25	0.0453±3.775E-03	0.0231±1.147E-03	0.51
FAD	y=0.14427x+0.0040854	0.9937	0.48	1.55	3.445E-02±2.863E-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+0.01668	0.9985	0.15	0.24	0.0844±7.021E-03	0.143±7.923E-03	1.69
Gamma-Aminobutyric acid	y=0.009372x+0.004264	0.9895	2.64	7.18	1.726±0.143	2.781±0.147	1.61
GDP	y=0.2184x-0.07534	0.9936	0.35	1.42	1.006E-04±8.367E-05	1.347E-04±6.621E-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
Gluconic 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
Glutaconic acid	y=0.02816x+0.00984	0.9913	0.57	1.71	0.0291±2.421E-03	0.0384±1.965E-03	1.32
Glutamic acid	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+0.0025903	0.9911	0.14	0.45	1.361±0.114	1.667±0.0788	1.22
Glyceraldehyde	y=0.4223x+0.0002	0.9948	2.48	7.44	4.696±0.395	4.546±0.292	0.97
Glyceraldehyde 3-phosphate	y=0.7085x+0.003266	0.9951	3.58	11.52	0.145±0.0121	0.152±7.353E-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±5.756E-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±5.112E-03	0.0601±3.123E-03	0.98
Glyoxylic 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	0.0278158±2.314E-03	0.0322±1.801E-03	1.16
Guanine	y=0.1883x+0.00004256	0.9971	0.13	0.55	7.251E-03±6.028E-04	5.559E-03±3.036E-04	0.77
Guanosine	y=0.01731x-0.008915	0.9968	0.59	1.32	0.132±0.0109	0.1142±0.0641	0.87
Hexose bisphosphate	y=1.165x+0.3801	0.9997	1.59	4.91	0.735±0.0612	0.471±0.0264	0.64
Hexose monophosphate	y=4.897x+0.1308	0.9998	1.62	3.68	0.119±9.905E-03	0.175±9.828E-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-0.0003355	0.9967	1.45	3.252	0.0483±3.182E-03	0.0712±4.003E-03	1.47
IDP	y=0.1543x-0.3808	0.9950	0.191	0.311	2.539E-03±2.111E-04	3.071E-03±1.612E-04	1.21
IMP	y=0.09851x-0.01637	0.9934	0.27	0.84	0.090±7.521E-03	0.108±6.414E-03	1.20
Inosine	y=0.4371x-0.00012982	0.9967	0.82	1.91	0.0712±5.931E-03	0.181±8.137E-03	2.54
Isoleucine	y=10.0409x+0.001933	0.9934	0.11	0.37	0.0967±8.051E-03	0.148±7.264E-03	1.53
ITP	y=0.1543x-0.3808	0.9972	0.079	0.21	2.684E-03±2.231E-04	3.488E-03±1.763E-04	1.30
Lactic acid	y=2.913x+0.0008827	0.9915	0.098	0.201	1.466±0.121	1.195±0.0618	0.82
Leucine	y=0.9814x-0.02699	0.9932	4.78	11.64	0.731±0.0606	0.6631±0.0346	0.91
Lysine	y=0.311x-0.0231	0.9907	5.09	15.57	0.0469±3.91E-03	0.0448±2.224E-03	0.96
LysoPC(16:0)	y=16.28192x+0.02058	0.9961	21.58	44.63	0.0158±1.321E-03	9.921E-03±4.89E-03	0.63
LysoPC(18:0)	y=12.0233x+0.006324	0.9970	21.51	44.93	0.353±0.0302	0.299±0.0138	0.85
LysoPC(22:0)	y=0.04398x+0.007898	0.9926	21.38	44.63	0.0641±5.462E-03	0.0495±2.287E-03	0.77
Malic acid	y=0.001268x+0.0005162	0.9988	0.075	1.13	3.878±0.322	4.157±0.225	1.07
Malonyl-CoA	y=0.001395x+0.0003158	0.9913	19.8	59.43	1.943E-04±1.618E-05	2.601E-04±1.269E-05	1.34
Methionine	y=1.2153x+0.03251	0.9926	3.28	12.61	0.627±0.0521	0.717±0.0361	1.14
Myoinositol	y=0.1005x+0.0001091	0.9917	7.21	18.66	0.0792±6.618E-03	0.0902±5.351E-03	1.14
N-Acetyl-glucosamine 1-phosphate	y=0.001781x+0.01991	0.9909	0.62	1.57	2.041E-03±1.705E-04	1.829E-03±9.017E-04	0.90
N-Acetylornithine	y=0.0383x+0.001343	0.9911	0.38	1.24	6.441E-04±5.362E-05	6.279E-04±3.512E-05	0.97
N-acetylserine	y=0.0697x+0.007435	0.9904	0.11	0.35	1.469E-04±1.22087E-05	4.137E-04±2.141E-05	2.82
NAD+	y=0.0839x+0.001167	0.9962	0.69	2.11	0.0255±2.121E-03	0.0161±8.834E-03	0.63
NADH	y=0.117x+0.003571	0.9999	0.047	0.197	3.039E-03±2.525E-04	4.524E-03±2.387E-04	1.49
NADP+	y=0.141x+0.0491	0.9957	0.057	0.18	0.0107±9.016E-04	7.718E-03±3.605E-04	0.72

NADPH	y=0.135x+0.0307	0.9944	0.052	0.19	0.0364±3.046E-03	0.0501±2.395E-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	7.336E-04±3.541E-05	1.17
Oleic acid	y=0.0202x+0.000432	0.9938	1.91	4.88	4.709E-04±4.006E-05	6.347E-04±4.441E-05	1.35
Ornithine	y=0.579x+0.0902	0.9995	2.17	6.05	0.116±9.664E-03	0.0898±4.839E-03	0.77
Orotidylic acid	y=1.503E-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	1.488±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±5.632E-02	2.53
PA(36:6)	y=0.05279x+0.002584	0.9997	2.31	5.55	0.0376±1.468E-03	0.0991±4.942E-03	2.64
p-Aminobenzoic acid	y=0.13576x+0.002926	0.9906	0.58	1.43	8.126E-03±6.757E-04	7.082E-03±3.959E-04	0.87
Pantothenic acid	y=0.1371x-0.03129	0.9900	0.079	0.25	2.912E-03±2.424E-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	1.82±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	3.019±0.251	2.792±0.157	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±06.067E-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(32:0)	y=0.6508x+0.04281	0.9937	5.82	9.63	0.843±0.0718	0.663±0.0305	0.79
PG(32:1)	y=0.6508x+0.04281	0.9937	5.82	9.63	0.435±0.0371	0.241±0.0167	0.55
PG(32:2)	y=0.6508x+0.04281	0.9937	5.82	9.63	ND	ND	ND
PG(34:1)	y=0.6508x+0.04281	0.9937	5.82	9.63	1.249±0.105	0.578±0.0391	0.46
PG(34:2)	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
Phenyllactic acid	y=0.05875x+0.05597	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±3.532E-05	0.88
Phosphoenolpyruvic acid	y=0.658x+0.001023	0.9944	1.14	4.21	0.0761±6.331E-03	0.0689±3.471E-03	0.91
Phosphoribosyl pyrophosphate	y=0.5684x-0.08531	0.9945	0.33	1.21	0.255±0.0212	0.242±0.0124	0.95
Phosphorylcholine	y=0.5219x+0.000007	0.9939	0.63	1.45	0.145±0.0121	0.161±0.0399	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±1.535E-03	0.88
Prephenate	y=0.01172x+0.1357	0.9999	0.13	0.29	1.549E-05±1.293E-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±2.073E-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±1.331E-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±2.841E-06	3.006E-05±1.516E-06	0.88
Pyroglutamic acid	y=0.01398x-0.002955	0.9915	0.079	0.23	8.38E-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=0.5335x+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	0.9991	0.37	1.35	0.112735±9.381E-03	0.295±0.0165	2.62
Riboflavin	y=0.08462x+0.0001534	0.9901	0.22	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	0.37	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-3.279	0.9999	1.99	4.23	0.725±0.0603	0.963±0.0505	1.33
Shikimic acid	y=5.404x+0.003765	0.9925	0.45	1.28	1.022E-04±8.511E-05	1.084E-04±5.338E-05	1.06
Spermidine	y=0.8305x+0.002175	0.9997	0.38	0.84	0.214±0.0178	0.352±0.0197	1.64
Succinic acid	y=1.9768x+0.04728	0.9982	0.056	0.19	0.128±0.0106	0.111±0.0559	0.87
Succinyl-CoA	y=0.01068x+0.003823	0.9983	0.11	0.23	8.201E-03±7.001E-04	6.241E-03±2.885E-04	0.76
Sucrose	y=0.03063x+0.0002063	0.9995	0.044	0.12	13.466±1.118	11.398±0.601	0.85
Thiamine	y=0.9425x+0.03937	0.9988	0.19	0.28	4.205E-04±3.501E-05	5.521E-04±2.721E-05	1.31
Thiamine monophosphate	y=0.2361x+0.006176	0.9937	0.11	0.36	1.489E-03±1.241E-04	1.374E-03±6.706E-04	0.92
Threonine	y=0.3018x-0.8278	0.9919	1.24	4.91	0.287±0.0239	0.743±0.0366	2.59
Thymidine	y=0.014x+0.00000712	0.9980	0.37	1.33	6.578E-03±5.481E-04	4.816E-03±2.341E-04	0.73

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±3.622E-05	1.21
Tyrosine	y=0.0013x+0.0000029	0.9920	2.68	5.77	2.339±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
Ureidosuccinic 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±0.0228	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