

Supplementary Table 5. Single reaction monitoring (SRM) transitions for metabolites measured in this study.

Compound name	Precursor ion	Product ion	Ionization
Nicotinamide-N-oxide	179.00	117/132	Positive
Gentisate (2,5-Dihydroxybenzoic acid)	155.03	137.02/98.9	Positive
Citrate	191.05	111/87	Negative
Malate	133.00	115/43/41	Negative
Guanosine	284.10	152/135	Positive
Retinoic acid (Vitamin B3)	301.10	161.3/123	Positive
1-Stearoyl-sn-glycero-3-phosphocholine	524.37	104.1 / 184.1	Positive
Oxaloacetate	131.00	87.00	Negative
Ergothioneine	230.10	127.03/186.1/60.05	Positive
Heptanoyl Carnitine	260.20	201.2/85	Positive
Benzene	78.00	52.00	Positive
Lactic acid	91.04	73/40.6	Positive
Myristoleic acid	227.20	43.1/41.2	Positive
AcetylcoenzymeA	810.15	303.1/135.9	Positive
Pyruvic acid	87.00	43.00	Negative
Aniline	94.07	77/51	Positive
Aminooctanoic acid	160.00	55.30	Positive
Nicotine imine	123.00	80.00	Positive
Methyl Nicotinamide	138.08	95.1/79.1	Positive
Acetylcholine	146.12	87.04/43.02	Positive
Cis Retinal	285.20	175.1/160.9	Positive
Isovaleryl Carnitine	246.20	85/187.1	Positive
4-Pyridoxate	182.04	138.20	Negative
Thymine	127.10	110.00	Positive
Octonyl Carnitine	288.20	85/57.1	Positive
Hydroxypalmitic acid, trimethylaminoethyl ester	269.00	47.00	Positive
Cotinine	177.10	98/80.1	Positive
Cyclophosphamide	261.00	106/120/140	Positive
Benzi(ghi)perylene	277.10	235.9/194.74	Positive
Aspartic acid	134.05	73.9/116	Positive
Nor nicotine	149.00	117/130	Positive
Xanthosine-5-phosphate	365.00	97.00	positive
Pyrene	203.00	202.00	Positive
AMP	348.07	97/136	Positive
GMP	364.07	152/135	Positive
4-Coumarate	165.04	119.00	Positive
Phospho Choline	185.08	99/87.1	Positive
UMP	191.05	111/87	Negative
Cytidine 5 -Monophosphate (5-CMP)	324.00	112/83.6	Positive
dCMP	308.06	112.00	Positive
Inositol-1P	371.01	158/234.9	Positive

Aminoimidazole carboxamide ribonucleotide	259.00	127/110/242	Positive
Aminobiphenyl	170.20	153.20	Positive
Creatinine	114.07	45/90/86.2	Positive
1-Methyl-Histidine	170.09	124.00	Positive
Methyl Adenosine	282.10	150/133	Positive
Nonadecanoic acid	298.29	281.40	Positive
Cystathionine	223.08	134.1/88.1	Positive
SAH	385.13	136.1/134	Positive
Methyl deoxyadenosine	252.00	136.00	Positive
S-Methyl-5-thioadenosine	298.00	136.00	Positive
Isobutyryl Carnitine	232.15	85/173	Positive
2-Methyl glutamic acid	162.08	116.10	Positive
Acetyl Carnitine	204.12	85.00	Positive
Betaine	118.09	58.1/59.2	Positive
Guanidine acetic acid	118.06	43.1/30.1	Positive
Homogentisate	167.03	122.9/107.8	Negative
Urea	61.00	44.00	Positive
Pantothenic acid	220.00	90.00	Positive
Glutathione, Reduced (GSH)	308.09	76/179	Positive
Indolacetaldehyde	160.08	142.066/130.03	Positive
Deoxy carnitine	146.12	87/60.1	Positive
Nicotinamide	179.00	117/132	Positive
Succinicacid	117.00	99/73	Negative
4 Hydroxybutyric acid	105.05	45.00	Positive
Ethylmalonate/Methyl Malonate	133.05	43.02/115.04	Positive
NAAG	305.10	148.2/84.1	Positive
5-Oxoproline	130.05	84.00	Positive
Homoserine	120.07	74.1/56.1	Positive
Allo-Threonine	120.07	56.1/74.1	Positive
Glutamic acid	146.00	128/102	Negative
Glycine	76.04	30.50	Positive
2-Aminobutyraldehyde	88.08	70.10	Positive
Glutamine	145.00	109/84	Negative
Aminohydantoin-nitrobenzaldehyde	249.10	134.00	Positive
ASP-PH	281.11	120.1/88/166.1	Positive
Iminoaspartate	132.03	114.02/86.02	Positive
Gly-Gly	133.06	30/76.04/42.03	Positive
Hydroxyglutaric acid	147.00	129.1/101.1/85	Negative
Tyrosine	182.08	136.1/91	Positive
Phenyl alanine	166.10	120.1/103.1	Positive
Valine	118.09	72.2/55	Positive
Isoleucine	132.10	86.1/43.9	Positive
Asparagine	133.06	87.1/74	Positive
Serine	106.05	88.1/60.1	Positive
Histidine	156.10	110.00	Positive
Methyl alanine	104.07	44/58.1	Positive
Choline	105.11	60.1/45	Positive

N, N Dimethyl Glycine	104.07	44/58.1	Positive
Methionine	150.06	61.1/56.1	Positive
Lysine	147.11	130.2/84.2	Positive
Citrulline	176.10	159/70.1	Positive
N-Acetylornithine	175.11	115/70.1	Positive
Arginine	175.12	60.2/70.1	Positive
Kynurenine	209.09	192/146	Positive
Tryptophan	205.10	188.1/146	Positive
NAD	664.12	428.2/136.1	Positive
NADH	666.13	428.2/136.1	Positive
NADP	742.00	620.00	Negative
NADPH	744.00	79.00	Negative

SRM transitions for Metabolic Flux

(AMP)	348.07	136.00	Positive
(AMP)(M+5)	353.07	136.00	Positive
(GMP)	364.07	152.00	Positive
(GMP)(M+5)	369.07	152.00	Positive
CMP	324.00	112.00	Positive
CMP(M+5)	329.00	112.00	Positive
IMP	349.00	137.00	Positive
IMP(M+5)	354.00	137.00	Positive
UMP	325.00	97.00	Positive
UMP(M+5)	330.00	97.00	Positive
G6P/F6P	259.02	96.90	Negative
G6P/F6P(m+6)	265.04	96.90	Negative
FBP/GBP	338.99	79.00	Negative
FBP/GBP(m+6)	345.01	79.00	Negative
Sedoheptulose-7-P	289.00	97.00	Negative
Sedoheptulose-7-P(m+7)	296.00	96.90	Negative
6-Phosphogluconate	275.00	96.90	Negative
6-Phosphogluconate (m+4)	279.00	96.90	Negative
Ribose/Ribulose/xylulose-5P	229.01	96.90	Negative
Ribose/Ribulose/xylulose-5P(m+5)	234.03	96.90	Negative
Erythrose-4-P	199.00	96.90	Negative
Erythrose-4-P(m+4)	203.00	96.90	Negative
Citrate	191.02	87.00	Negative
Citrate(m+2)	193.03	112.00	Negative
Malic acid	133.01	71.01	Negative
Malic acid(m+2)	135.02	117.00	Negative
Succinic acid	117.02	73.00	Negative
Succinic acid (m+2)	119.03	74.00	Negative
Kynurenine	209.10	146.00	Positive
Kynurenine(M+2)	211.10	148.00	Positive