

Table S1. Instrumentation setup for the targeted metabolites in this study

Compound	Retention Time (min)	Polarity	Precursor (m/z)	Product1 (m/z)	Product2 (m/z)	Collision Energy1 (V)	Collision Energy2 (V)	RF Lens (V)
paraxanthine	1.35	Positive	181.213	108.9	124.1	10.253	20.9	84
2,4-dihydropyrimidine-5-carboxylic acid	1.5	Positive	157.091	116.1	139	10.253	12.5	45
deoxyribose	1.12	Positive	135.122	94.06	107	10.253	10.3	56
alpha-hydroxyisobutyric acid	1.13	Positive	105.122	51.1	77.04	27.191	10.3	82
uridine 5'-diphosphate	1.13	Positive	405.122	388.5		10.253		81
galactarate	1.16	Positive	211.122	175.1	193.2	11.82	10.3	51
lauroylcarnitine	1.17	Positive	344.243	84.99	285	22.742	15.9	94
2'-deoxyguanosine	1.19	Positive	286.183	214	268	15.764	18	70
dihydroxyacetone phosphate	1.2	Positive	183.152	105.1	165.1	14.753	10.3	52
glycolaldehyde dimer	1.21	Positive	121.122	77.11	103.1	20.871	10.3	49
D-glucose 6-phosphate	1.21	Positive	261.183	129	189.1	16.169	10.3	75
D-ribose 1,5-bisphosphate	1.21	Positive	311.183	101.2	221.1	10.253	14.4	71
glutaric acid	1.22	Positive	133.122	105.2	115.1	15.258	10.3	37
ethanolamine phosphate	1.23	Positive	142.639	85.11	125.1	11.567	10.3	44
inosine	1.23	Positive	268.939	180.9	252.9	46.404	25.9	249
homocystine	1.23	Positive	268.97	180.9	252.9	45.545	24.9	249
isopentyl pyrophosphate	1.23	Positive	298.03	205.8	282.1	55	10.3	58
thiamine monophosphate	1.23	Positive	345.122	84.9		18.697		88
shikimate	1.25	Positive	175.122	119.1	147.1	16.219	14	56
tetrahydrofolate	1.25	Positive	446.091	341.9	430.1	15.713	11.1	77
3-hydroxybutanoic acid	1.27	Positive	105.104	73.11	87.11	10.253	10.3	30
D-glyceric acid	1.28	Positive	107.043	79.05	89.06	10.253	10.3	41
trans-aconitate	1.28	Positive	175.152	73.18	143.1	10.253	10.3	30
mevalolactone	1.3	Positive	131.122	69.11	113.1	10.253	10.3	46
inosine 5'-diphosphate	1.3	Positive	429.03	340.2		18.09		132
indoxyl sulfate	1.32	Positive	134.122	93.06	106.1	10.253	14.6	93

D-lactose	1.32	Positive	361.03	343	352	10.253	10.9	84
caffeine	1.35	Positive	195.152	110.1	138.1	22.944	19.6	81
theophylline	1.38	Positive	181.061	124.1	163.1	19.152	10.3	58
formate	1.39	Positive	47.213	15.44	31.22	18.09	10.3	65
methylguanidine	1.4	Positive	74.152	33.22	42.22	13.489	10.3	30
N-acetyl-D-tryptophan	1.41	Positive	247.152	159.1	201.1	18.292	11.4	46
5'-methylthioadenosine	1.41	Positive	298.091	136.1	163	17.685	10.3	66
1,3-diaminopropane	1.42	Positive	75.061	43.18	57.11	10.253	10.3	66
aniline-2-sulfonic acid	1.42	Positive	174.03	92.11	156.1	16.978	10.3	55
thymine	1.44	Positive	127.304	84.04	110.1	15.865	15.9	62
glycerol	1.45	Positive	93.122	43.22	61.11	10.253	10.3	30
nicotinamide	1.45	Positive	123.122	78.11	80.11	23.197	20.2	68
theobromine	1.45	Positive	181.152	138	163.1	17.129	16	85
thymidine	1.45	Positive	243.122	117	127.1	10.607	10.3	31
2-deoxy-D-glucose	1.46	Positive	165.639	129	148.1	22.539	18.4	55
thiourea	1.5	Positive	77.122	43.15	60.04	35.888	18	43
nicotinate	1.5	Positive	124.091	96.11	106.1	11.315	10.3	53
5'-deoxyadenosine	1.51	Positive	252.122	119	136	45.039	15.5	54
trigonelline	2.02	Positive	138.122	92.11	120	19.354	10.3	66
D-pantothenic acid	1.52	Positive	220.152	90.11	202	10.253	13	53
formyl-L-methionyl	1.53	Positive	178.122	104.1	130	16.32	11.3	58
purine	1.54	Positive	121.122	67.11	94	28.455	20.7	102
2,4-dihydroxypteridine	1.57	Positive	165.152	120.1	148	20.517	15.5	77
S-hexyl-glutathione	1.58	Positive	392.183	246	263	14.298	11.1	75
riboflavin	1.63	Positive	377.152	198	243	35.736	22.1	112
uridine	1.65	Positive	245.152	113.1	117	10.253	10.3	48
coenzyme A	2.16	Positive	768.152	428.1		22.792		113
urocanate	1.68	Positive	139.152	91.13	111	17.129	10.3	57
adenosine	1.68	Positive	268.122	119	136.1	46.253	19.1	70
D-(+)-glucosamine	1.69	Positive	180.152	139.2	163.1	11.871	10.3	43
D-glucono-1, 5-lactone	1.73	Positive	179.15	119.1	161	13.236	11	62

3',5'-cyclic AMP	1.73	Positive	330.091	136	312	23.803	17.3	84
3-ureidopropionate	1.74	Positive	133.122	90.1	115	10.253	10.3	43
adenosine 3',5'-cyclic monophosphate	1.75	Positive	329.983	136.1	312	24.815	16.8	87
tryptophan	1.78	Positive	205.15	146	188	18.242	12.6	64
L-kynurenine	1.78	Positive	209.152	94.11	192	15.966	10.3	57.7
D-tryptophan	1.8	Positive	205.152	146	188.1	15.764	10.8	41
norleucine	1.81	Positive	132.152	69.11	86.17	15.663	11.9	30
isoleucine	1.81	Positive	132.152	69.18	86.18	16.674	10.3	40
leucine	1.81	Positive	132.152	86.11	114.1	10.253	10.3	47
6'-hydroxynicotinate	1.82	Positive	140.122	94.04	122.1	21.983	17.6	86
N-acetyl-DL-glutamic acid	1.83	Positive	190.183	84.11	130.1	22.792	12.3	47
N-alpha-acetyl-L-lysine	2.35	Positive	189.152	84.11	129.1	21.781	14	53
phenylalanine	1.86	Positive	166.15	103.1	120.1	27.65	13.8	54
deoxycytidine	1.86	Positive	228.152	94.99	112	35.079	10.3	30
5-oxo-D-proline	1.89	Positive	130.122	84.04	102	10.253	10.3	57
acetylcholine	1.89	Positive	147.152	87.04	88.11	13.64	10.3	51
N-alpha-acetyl-L-asparagine	1.9	Positive	175.152	133		10.556		65
N-acetyl-L-cysteine	1.91	Positive	163.122	43.22	121.1	16.876	10.3	57
pyrazole	1.92	Positive	67.97	40.17	41.17	10.253	18.6	115
cytidine	1.93	Positive	244.152	95.06	112.1	40.893	16.3	46.8
SN-glycero-3-phosphocholine	2.43	Positive	259.183	105.1	125	15.157	26.9	79
cytidine 2'3'-cyclic monophosphate	1.93	Positive	306.03	112	177.9	15.461	19.1	61
methionine	1.95	Positive	150.122	104.1	133	11.112	10.3	46
D-glucuronoactone	1.95	Positive	177.274	121.1	149.1	15.865	12.8	72
N-acetyl-D-glucosamine	1.95	Positive	222.304	144.2	167.9	17.685	10.3	55.7
maleimide	1.96	Positive	98.152	57.11	70.11	10.253	13.9	44
selenomethionine	1.96	Positive	198.183	109	180.9	24.107	11.9	43
creatinine	1.97	Positive	114.122	44.22	86.11	17.281	11.3	38
3-hydroxykynurenine	1.97	Positive	225.152	162.1	208.1	19.253	10.3	57
N-acetyl-D-galactosamine	1.98	Positive	222.152	126.1	204.1	12.983	10.3	35
5-methylcytosine hydrochloride	2	Positive	126.152	108	109	18.949	20.1	88

uridine-5-monophosphate	2	Positive	325.183	185.1	307.2	26.382	12.4	79
5-aminoimidazole 4-carboxamide-1-beta-D-ribofuranosyl-5'-monophosphate	2.5	Positive	339.061	127.1	206	12.478	10.3	65
cytosine	2.02	Positive	112.3	69.11	95.05	16.775	21.5	72
5-hydroxy-L-tryptophan	2.02	Positive	221.152	162.1	204	19	11	52
citramalate	2.03	Positive	149.122	93.06	121.1	17.635	15.8	73
Betaine	2.04	Positive	118.152	58.17	59.17	23.399	19	80
proline	2.05	Positive	116.152	70.11	88.11	12.831	13.2	56
taurine	2.06	Positive	126.122	81.05	108	16.067	10.3	53.7
O-acetyl-L-serine	2.07	Positive	148.091	113	131.1	10.253	10.3	30
N-acetylneuramate	2.07	Positive	309.726	255.2	292	16.573	10.3	70
tyrosine	2.08	Positive	182.15	136.1	165	10.25	11.4	40
adenosine 5'-monophosphate	2.08	Positive	348.183	136.1		23.146		73
inosine 5'-monophosphate	2.58	Positive	349.122	137.1		13.893		78
valine	2.1	Positive	118.152	72.11	100.1	13.691	13.4	56
guanine	2.11	Positive	152.243	123.9	134	16.27	13.5	84
pyridoxine	2.11	Positive	170.03	134	151.9	20.669	12.3	52
O-succinyl-L-homoserine	2.12	Positive	220.122	102.1	120	11.416	13.8	60
pipecolate	2.14	Positive	130.122	84.11	102.1	12.933	10.4	53.2
maleamate	2.15	Positive	116.122	72.17	88.11	12.831	13.3	53
D-aspartate	2.15	Positive	134.152	86.11	116.1	19.202	10.3	48.5
5,6-dihydrouracil	2.16	Positive	115.122	42.22	74.11	10.253	10.3	30
cysteine	2.17	Positive	122.122	59.04	76.06	22.135	13.1	34
hypotaurine	2.18	Positive	110.091	82.13	92.06	12.427	10.3	58
ophthalmic acid	2.19	Positive	290.139	161.1	215	12.478	10.3	68
S-carboxymethyl-L-cysteine	2.2	Positive	180.122	117.1	163	15.208	10.3	53
galactitol	2.21	Positive	183.122	129	165.1	10.253	10.3	56
glycolate	2.22	Positive	77.152	45.17	59.11	10.253	10.3	36.9
(2R,3R)-(-)-2, 3-butanediol	2.22	Positive	91.122	50.17	65.11	10.253	19.7	98
alpha-aminoadipate	2.22	Positive	162.243	108.9	127	32.702	20.3	75
4-hydroxy-L-proline	2.23	Positive	132.152	90.04	114.1	13.388	10.3	48

trans-4-hydroxyproline	2.23	Positive	132.274	68.05	86.13	21.124	11.7	34
4-hydroxy-L-phenylglycine	2.23	Positive	168.122	123.1	151.1	18.14	10.3	30
kynurenine	2.23	Positive	209.152	179	193	21.68	19.4	102
glutathione	2.23	Positive	308.304	162.1	179.1	14.955	10.8	77
glycine	2.24	Positive	76.373	42.17	58.1	10.253	10.3	30
mesoxalate	2.24	Positive	119.122	91.11	101.2	15.713	10.3	53
cis-4-hydroxy-D-proline	2.24	Positive	132.122	68.11	86.11	22.388	10.3	52
alanine	2.25	Positive	90.122	44.15	62.11	10.253	10.3	30
2-amino-2-methylpropanoate	2.25	Positive	104.122	45.15	58.17	10.253	11.4	30
3-aminoisobutanoate	2.25	Positive	104.152	30.29	86.11	12.781	10.3	30
diethanolamine	2.25	Positive	106.152	70.11	88.11	10.253	11	30
N-acetyl glycine	2.25	Positive	118.152	72.09	100	16.32	13.1	59
L-norvaline	2.25	Positive	118.152	72.11	100.1	15.764	13.9	59
L-homocysteine thiolactone	2.25	Positive	118.152	90.07	100	10.253	13.7	55
N-amidino-L-aspartate	2.25	Positive	176.122	88.06	134	14.854	10.3	59
N-acetyl-DL-serine	2.26	Positive	148.087	60.1	106.1	16.775	10.3	31
ethyl 3-ureidopropionate	2.26	Positive	161.122	92.06	120	13.236	10.3	56
DL-normetanephrine	2.26	Positive	184.152	134.1	166.1	19.556	10.3	34
glyceraldehyde	2.27	Positive	91.152	63.04	65.11	27.697	20.5	131
5-aminolevulinic acid	2.27	Positive	132.091	90	114.1	10.253	11.3	46
2-aminoethyl dihydrogen phosphate	2.27	Positive	142.122	42.22	83.11	12.73	10.3	30
3-sulfinyl-L-alanine	2.27	Positive	154.122	106.1	122	14.551	10.3	63
adenosine 5'-diphosphoribose	2.27	Positive	560.152	348	428.1	14.652	20.3	91
1-methylnicotinamide	2.28	Positive	138.152	93.1	95.06	21.174	19.6	78
4-guanidinobutanoate	2.28	Positive	146.152	86.06	87.04	15.865	13.4	57
octopamine	2.28	Positive	154.152	113.1	136	10.253	10.3	45
noradrenaline	2.28	Positive	170.183	93.04	152	26.129	10.3	83
epinephrine	2.28	Positive	184.087	166		11.213		61
D-(+)-galacturonic acid	2.28	Positive	213.152	113.2	121.1	14.449	11.6	57
N-formylglycine	2.29	Positive	104.152	45.15	63.1	17.079	10.3	50
choline	2.29	Positive	105.122	51.11	77.11	27.292	10.3	75

N-acetylputrescene	2.29	Positive	131.152	72.17	114.1	15.461	10.3	48
dopamine	2.33	Positive	154.152	91.18	137.1	21.781	12.7	46
D-alanine	2.34	Positive	90.152	44.22	45.22	11.011	10.3	42
ethanolamine	2.35	Positive	62.152	44.18	46.11	12.376	34.2	51
creatine	2.36	Positive	132.122	86.11	114.1	10.253	10.3	39
4-aminobutanoate	2.38	Positive	104.122	86.05	87.13	10.657	10.4	46.8
5-aminopentanoate	2.39	Positive	118.152	55.15	101.1	16.421	10.3	52
homoserine	2.39	Positive	120.122	56.11	74.11	17.028	10.3	41
threonine	2.39	Positive	120.122	74.11	102.1	10.253	10.3	41
L-carnitine	2.39	Positive	162.122	85.07	103	20.517	17	78
Beta-Alanine	2.43	Positive	90.152	45.15	72.11	10.253	10.3	40.6
L-allothreonine	2.43	Positive	120.122	60.1	102.1	10.253	10.3	41
glutamine	2.45	Positive	147.152	84.11	130	18.242	11.8	62
4-imidazoleacetic acid	2.46	Positive	127.152	81.04	109	16.522	10.3	47
guanidinoacetate	2.49	Positive	118.152	72.18	100.2	15.865	13.5	56
deoxycarnitine	2.51	Positive	146.152	60.17	87.04	13.843	15.7	57
hydroxypyruvate	2.57	Positive	105.152	63.13	64.07	10.253	10.3	30
2-hydroxybutyric acid	2.6	Positive	105.122	23.33	64.04	10.253	10.3	30
L-anserine	2.61	Positive	304.061	214.9	244.9	15.157	14.9	87
thymidine 5'-monophosphate	2.63	Positive	323.122	202	282	15.107	10.3	43
histamine	2.64	Positive	112.152	68.11	95.11	19.758	11.1	52
inosine 5'-triphosphate	2.66	Positive	508.939	262.9	344.9	24.612	10.3	89
asparagine	2.67	Positive	133.122	74.04	87.11	15.612	10.3	36
L-methionine sulfoximine	2.67	Positive	181.061	74.11	102.1	14.904	10.3	38
cytidine 5'-diphosphocholine	3.2	Positive	490.183	264.9	379	25.927	13	103
L-histidinol	2.71	Positive	142.152	81.04	124.2	19.506	10.4	52
serine	2.74	Positive	106.15	60.11	88	10.25	10.3	42
alpha-D-glucose 1-phosphate	2.82	Positive	261.087	163.1	242.9	10.253	10.3	59
D-glucosamine 6-sulfate	2.84	Positive	260.174	162	242.1	10.657	11	53
2-acetamido-2-deoxy-beta-D-glucosylamine	2.86	Positive	221.152	138.1	161	16.674	11.5	55
pyridoxamine	2.87	Positive	169.122	134.1	152.1	22.135	11.7	30

glutamic acid	2.95	Positive	148.152	84.2	130.3	15.006	10.9	45
3-methylhistamine	2.96	Positive	126.152	96.13	109.2	21.022	16.4	62
histidine	3.15	Positive	156	83.02	110.1	23.348	12.1	49
D-mannosamine	3.29	Positive	180.152	83.99	162.1	15.107	11.5	33
aspartic acid	3.34	Positive	134.243	59.04	87.99	26.331	10.3	40
O-phospho-DL-serine	4	Positive	186.152	88.13	145.1	10.253	10.3	54
D-(+)-galactosamine	3.51	Positive	180.087	152.1	162.1	10.253	12.4	64
stachyose	4.02	Positive	667	416.9		15.612		115
glucosaminat	3.53	Positive	196.152	132	178.1	13.691	10.3	68
NAD	3.53	Positive	664.152	428	444	25.725	25.5	99
nepsilon, nepsilon, nepsilon-trimethyllysine	3.7	Positive	189.183	84.11	130.1	20.567	13.7	70
carnosine	3.76	Positive	227.122	192.9	209.1	26.23	10.3	66
homocysteine	3.8	Positive	136.091	89.97	91.04	10.91	18.8	65
arginine	3.85	Positive	175.152	70.11	116	21.579	10.3	64
lysine	3.94	Positive	147.122	84.02	130.2	15.612	13.1	43
agmatine sulfate	4.03	Positive	130.97	89.11	113.1	10.253	10.3	35
L-ornithine	4.36	Positive	133.122	70.04	116.1	18.697	10.3	38
D-orinthine	4.36	Positive	133.152	105.1	115.1	15.511	11.7	47
L-2, 3-diaminopropionic acid	4.54	Positive	105.122	64.11	88.11	10.253	10.3	30
cystine	4.7	Positive	241.304	120	151.9	18.393	12.7	59
DL-5-hydroxylysine	4.85	Positive	163.152	128	145.2	10.253	10.3	53
D-glucosamine 6-phosphate	5.28	Positive	260	126.1	144.1	10.253	14.7	72
phosphocholine	5.8	Positive	184.091	86.18	125	16.775	19.2	62
dihydroxyfumaric acid	1.22	Negative	165.122	149		16.27		60
phospho(enol) pyruvic acid	1.5	Negative	167.03	78.97	83.1	10.253	11.2	0
(S)-malate	1.68	Negative	133.061	71.16	115.1	10.253	10.3	0
N-acetyl-DL-methionine	1.28	Negative	190.183	141.9	147.9	15.36	12.4	0
N-acetyl-L-alanine	1.34	Negative	129.97	88.18		12.174		53
(R)-malate	1.67	Negative	133.091	73.11	115.1	17.331	16.5	44
isocitric acid	1.79	Negative	191.122	85.08	111.1	11.011	13.5	0
pyridoxal 5'-phosphate	1.99	Negative	263.974	99		19.607		59

gluconic acid	2	Negative	195.274	75.17	99.1	17.685	18.8	0
3'-CMP	2.5	Negative	322.091	110.1	211	26.028	17.6	72
(S,S)-tartaric acid	2.17	Negative	148.97	73.05	87.11	16.624	10.6	52
thymidine-5'-diphospho-alpha-D-glucose	2.23	Negative	563.091	241	321.1	30.275	22.3	121
D-fructose 6-phosphate	2.27	Negative	258.991	79.06	97	38.163	14.7	65
xanthosine 5'-monophosphate	2.27	Negative	363.009	151.1	211	27.191	18.3	83
folic acid	2.33	Negative	440.183	311.1	396.1	22.084	23.1	105
D-mannose 6-phosphate	2.75	Negative	258.991	97	199	15.006	12.6	61
L-cystathionine	4.1	Negative	221.122	120.1	134.1	11.972	11.1	58
D-ribulose 1,5-bisphosphate	5.17	Negative	308.939	97.07	211.1	18.697	12.5	69
