

## Supplementary Table1-List of Metabolites targeted in the samples

Compound Name	Precursor Ion	Product Ion	Polarity
Urea	61.0396	44	Positive
Glycine	76.0393	30.5	Positive
2-Aminobutyraldehyde	88.0757	70.1	Positive
Pyruvate	88.2	42.2	Positive
Putrescine	89.1073	72.1	Positive
sarcosine	90.055	44.1	Positive
Alanine	90.06	72.1	Positive
Lactic acid	91.04	73	Positive
2-Hydroxypyridine	96.0444	51.1	Positive
betaine aldehyde	103.0992	58	Positive
4-aminobutyrate	104.0706	69	Positive
Aminobutyric acid	104.0706	44.1	Positive
Methyl alanine	104.0706	58.1	Positive
N, N Dimethyl Glycine	104.0706	58.1	Positive
4 Hydroxybutyric acid	105.0546	45	Positive
Choline	105.1148	60.1	Positive
Serine	106.0499	88.1	Positive
Histamine	112.0869	95.1	Positive
Cytosine	112.1	95.1	Positive
Uracil	113	72	Positive
Creatinine	114.0662	90	Positive
Proline	116.0706	70.1	Positive
Guanidine acetic acid	118.0611	30.1	Positive
Betaine	118.0863	59.2	Positive
Valine	118.0863	55	Positive
D-Erythronic acid $\gamma$ -lactone	119.11	91.1	Positive
Allo-Threonine	120.0655	74.1	Positive
Homoserine	120.0655	74.1	Positive
Theronine	120.0655	56.1	Positive
purine	121.0509	94	Positive
Cysteine	122.027	59	Positive
Nicotinamide	123.0553	80.1	Positive
Thymine	127.0502	110	Positive
5-oxo-proline	130.0499	84	Positive
DL-Pipecolic acid	130.0863	84	Positive
4-Methyl-2-oxo pentanoic acid	131.0703	43.06	Positive
L-Thymine	131.1	113.9	Positive
N-Acetylputrescine	131.1179	114	Positive
Hydroxyglutaric acid	132	45	Positive
N-acetylalanine	132.0655	90.05	Positive
Isoleucine	132.1019	43.9	Positive
Ethylmalonate/Methyl Malonate	133.0495	115.04	Positive
Asparagine	133.0608	87.1	Positive
Gly-Gly	133.0608	30	Positive
Homocysteine	136.05	90	Positive

Adenine	136.6	119	Positive
Hypoxanthine	137	119	Positive
Methyl Nicotinamide	138.08	95.1	Positive
4 AcetamidoBA	146.08	86.1	Positive
2-Aminoheptanoic acid	146.1176	100.1	Positive
Acetylcholine	146.1176	43.02	Positive
Deoxy carnitine	146.1176	60.1	Positive
Spermidine	146.1652	112.1	Positive
Methylglutaric acid	147.065	59.049	Positive
Lysine	147.1128	84.2	Positive
Glutamic acid	148.0604	84	Positive
Xanthine	153.04	136	Positive
Histidine	156.0768	83	Positive
3-Indoleacetonitrile	157.08	130.1	Positive
2-Aminooctanoic acid	160.1332	55.3	Positive
Carnitine	162.1125	60.1	Positive
4-Coumarate	165.0446	119	Positive
Phenyl alanine	166.0963	103.1	Positive
Phenylalanine	166.0963	120.1	Positive
1-Methyl-Histidine	170.0924	124	Positive
Glycerol 3-phosphate	173.02	132	Positive
Gly-Pro	173.0921	116.1	Positive
Suberic acid	175.1	157.1	Positive
N-Acetylorithine	175.1077	70.1	Positive
Arginine	175.119	60.2	Positive
citrulline	176.103	159	Positive
N-carbamoyl-L-aspartate	177.0506	74	Positive
L-Arginine	177.1	159.1	Positive
Glucosamine/Galactosamine	180.0866	162	Positive
Tyrosine	182.0812	91	Positive
Phospho Choline	185.0811	99	Positive
3-phospho-serine	186.0162	88	Positive
N-acetyl-glutamine	189.087	130	Positive
Gly-Leu	189.1234	171	Positive
N-Acetyl Lysine	189.1234	129	Positive
N-Acetyl Methionine	192	104.1	Positive
Quinic acid	193.0707	129.05	Positive
Aminophosphovaleric acid	198.0625	86.1	Positive
Dimethyl Arginine	203.1503	70.1	Positive
Spermine	203.23	112.1	Positive
Acetyl Carnitine	204.123	85	Positive
Tryptophan	205.1	188.1	Positive
Kynurenine	209.0921	192	Positive
Propeonyl Carnitine	218.1387	85	Positive
Glutamyl alanine	219.1	84.1	Positive
1methyl tryptophan	219.1128	202.1	Positive
Cystathionine	223.0747	134.1	Positive

3-Hydroxykynurenine	225.087	162.1	Positive
Myristoleic acid	227.2006	43.1	Positive
Myristic acid	229	38.9	Positive
Pyroglu-Va	229.1183	183.11	Positive
Ergothioneine	230.0958	186.1059	Positive
Isobutyryl Carnitine	232.1543	173	Positive
Cystine	241.03	74.1	Positive
Isovaleryl Carnitine	246.2	187.1	Positive
MYRISTATE (14:0)+Na	250	173	Positive
Palmitic acid	257	57	Positive
acadesine	259.1037	110	Positive
D-glucosamine-1-phosphate	260.053	162.1	Positive
Heptanoyl Carnitine	260.2	201.2	Positive
Glu-Leu	261.1445	187	Positive
thiamine	266.1196	122	Positive
S-ribosyl-L-homocysteine_pos	268.0849	88	Positive
Glu-Glu	277.103	148.06	Positive
ASP-PH	281.1132	166.1	Positive
Methyl Adenosine	282.1	150	Positive
Oleic acid	283.27	89.2	Positive
Guanosine	284.0989	135	Positive
Octonyl Carnitine	288.2	85	Positive
L-arginino-succinate	291.1299	70	Positive
Aspartame	295.1288	180.1	Positive
Phe-Glu	295.12889	120.08	Positive
10-NONADECENOATE (19:1N9)	297.2788	281.4	Positive
7-methylguanosine	299.1224	166	Positive
N-acetyl Glucosamine 6 Phos	302.0635	284.1	Positive
NAAG	305.0979	148.2	Positive
dCMP	308.0642	112	Positive
Glutathione, Reduced (GSH)	308.0911	76	Positive
N-Acetylneuraminic acid	310.1	274.1	Positive
Glu-Tyr	311.1238	247.1	Positive
Hydroxy Stearic acid Methy este	315.3	97.1	Positive
Cytidine 5 -Monophosphate (5-C	324.0591	112	Positive
UMP	325.0431	113.03	Positive
1,5-ANHYDROGLUCITOL (1,5-AG	329	165	Positive
cyclic AMP	330.06	136	Positive
Nicotinamide ribotide	335	123	Positive
aminoimidazole carboxamide rib	339.07	110	Positive
AMP	348.0704	136	Positive
dGMP	348.0704	135	Positive
GMP	364.0653	152	Positive
3.alpha.-Mannobiose	343.1217	343.1217	Positive
1-Methylnicotinamide cation	138.0556	138.0556	Positive
.beta.-D-Glucose	198.097	198.097	Positive
L-Cystine	241.0314	241.0314	Positive

L-Sorbose	163.06	163.06	Positive
Docosaheptaenoic acid ethyl ester	357.2779	357.2779	Positive
Lactose	343.1229	343.1229	Positive
14(15)-EpETE	301.1427	301.1427	Positive
Chenodeoxycholic acid	357.2771	357.2771	Positive
3,4,5-Trimethoxycinnamic acid	239.1585	239.1585	Positive
6-Keto Testosterone Enanthate	285.204	285.204	Positive
Arachidonoyl amide	305.1565	305.1565	Positive
Isomyristic acid	229.2158	229.2158	Positive
Zearalenone	302.1225	302.1225	Positive
6-Ketoprostaglandin E1	351.1009	351.1009	Positive
N-Nervonoyltaurine	110.0095	110.0095	Positive
Lithocholic acid	358.2065	358.2065	Positive
Pentadecanoic acid, 14-methyl-	257.2473	257.2473	Positive
Idebenone	261.1294	261.1294	Positive
15(S)-15-Methylprostaglandin E1	314.9497	314.9497	Positive
Difloxacin	382.9303	382.9303	Positive
Sedoheptulosan	191.0169	191.0169	Positive
2-Chloro-L-phenylalanine	200.0408	200.0408	Positive
2',3,4,5,6'-Pentamethoxychalcone	341.092	341.092	Positive
D-myo-Inositol-1-phosphate	261.0381	261.0381	Positive
Dihydrocodeine	302.023	302.023	Positive
3-Hydroxy-3-methylglutaric acid	160.0774	160.0774	Positive
11-Dehydrothromboxane B2	351.0993	351.0993	Positive
Trifluoroacetic acid	115.0384	115.0384	Positive
Hydroxyflutamide	276.1431	276.1431	Positive
2-(14,15-Epoxyeicosatrienoyl)glycerol	303.0764	303.0764	Positive
Bis(2-ethylhexyl) phthalate	390.9789	390.9789	Positive
Resorcinol sulfoxide	246.2101	246.2101	Positive
4,6-Dimethyl-3,7-di(4-methoxyphenyl)pyridine	454.0327	454.0327	Positive
3,4'-Dihydroxyflavone	255.1945	255.1945	Positive
Nadolol	310.1463	310.1463	Positive
15-HETE	303.0855	303.0855	Positive
3-Ethoxy-1-propanol	126.5279	126.5279	Positive
17-Phenoxyprostaglandin F2.alpha.	351.1012	351.1012	Positive
3-Cyclopentyl-1-propanol	110.0103	110.0103	Positive
Prothioconazole	327.2001	327.2001	Positive
7-Methoxyloxapine	357.956	357.956	Positive
Butorphanol	310.1445	310.1445	Positive
1-Oleoyl-L-.alpha.-lysophosphatidylcholine	110.0103	110.0103	Positive
3-Hydroxy-3-methylglutaryl-CoA	912.2	428	Positive
1,3-diphosphatidylglycerate	265	79	Positive
2,3-dihydroxybenzoic acid	153	109	Positive
3PG and 2PG	184.9	97	Positive
3-phosphoglycerate	185	97	Positive
6-phospho-D-gluconate	275	97	Positive
acetylphosphate	139	79	Positive

ADP_neg	426.1	159	Positive
allantoin	157.05	114	Positive
anthranilate	136	92	Positive
cholesteryl sulfate	465.2	97	Positive
Cholesterol	385.3	217.7	Positive
dGDP_neg	426.12	159	Positive
dihydroorotate	157	113	Positive
D-sedoheptulose-1-7-phosphate	289	97	Positive
Farnesyl-PP	381	78.7	Positive
FBP/GBP	338.9	96.8	Positive
Fructose-6-Phosphate	259	97.1	Positive
Fumaric acid	115	71.1	Positive
Glucose-6-Phosphate	259	97	Positive
Glucuronic acid	193	113	Positive
Glutamine	145	109	Positive
glycolate	75	45.2	Positive
HBA	103	59.1	Positive
hexose-phosphate	259	79	Positive
Hydroxyisocaproic acid	131.006	85.1	Positive
inosine	267	135	Positive
Ketoglutarate	145	101.1	Positive
lactate	89	43.2	Positive
L-Anthranilic acid	137	93	Positive
L-Gibberilic acid	345	143	Positive
L-Jasmonic acid	209	126.9	Positive
L-Threonic acid	135	75.1	Positive
Malic acid	133	115.1	Positive
Malonate (Propanedioate)	103.1	59.1	Positive
Maltose	341.1	161	Positive
MALTOTETRAOSE	665.2	161.1	Positive
NAD+_neg	662	540	Positive
N-Aetyl Aspartic acid	174	88.1	Positive
Octanoic acid	143.1	125.1	Positive
octulose-monophosphate (O8P-	319	97	Positive
p-aminobenzoate	136.05	92	Positive
PEP	167	79	Positive
Ribose-5-phosphate	229.01	138.98	Positive
shikimate	173	93	Positive
S-ribosyl-L-homocysteine_neg	266	134	Positive
Stearic acid	283.48	265.2	Positive
succinate	117	73	Positive
Succinic acid	117	99.9	Positive
taurine	124	80	Positive
trehalose-6-Phosphate	421	79	Positive
UDP-D-glucose	565	323	Positive
UDP-D-glucuronate	579	403	Positive
UDP-N-acetyl-glucosamine	606	385	Positive

Uric acid	167.001	124	Positive
uridine	243	200	Positive
Sarcosine/Alanine	90.04	44.1	Positive
N, N Dimethyl Glycine/Methyl al	104.1	58.1	Positive
5-Hydroxyindolacetic acid	192.0655	146	Positive
2-Methylbutyrylcarnitine	246	187	Positive
2 Methyl glutamic acid	162.1	116.1	Positive
Hydroxy kynurinine	225.1	162.1	Positive
Erythrono-1,4-lactone	119.11	91.1	Positive
Acetyl Methionine	192.1	61	Positive
Amino phosphovelureic acid	198.1	135	Positive
Lauric acid	201.2	114.8	Positive
Ethyl 3 Indoleacetate	204.1	130	Positive
Carnitine, butyl ester	218	103	Positive
Citrate	191.05	111	Negative
D-glyceraldehyde-3-phosphate	169.05	97	Negative
GlucoseFructose	179	59	Negative
Hydroxy glutarate	147	129.1	Negative
Methylmalonic acid	117.002	73.1	Negative
orotate	155	111	Negative
Ribose	149	65	Negative
dihydroxy-acetone-phosphate	169	79	Negative
Glycerol 3 Phosphate	171	97	Negative
sn-glycerol-3-phosphate	171	79	Negative
aconitate	173.05	85	Negative
allantoate	175	132	Negative
Ascorbic acid	175.001	87	Negative
2-Isopropylmalic acid	175.002	115	Negative
N-carbamoyl-L-aspartate_neg	175.03	132	Negative
Pyrophosphate	176.8	158.6	Negative
glucono-D-lactone	177	129	Negative
myo-inositol	179	161	Negative
hydroxyphenylpyruvate	179.05	107	Negative
Indoleacrylic acid	186	142.03	Negative
Kynurenic acid	188	144	Negative
citrate-isocitrate	191	111	Negative
2-dehydro-D-gluconate	193	103	Negative
D-gluconate	195	129	Negative
D-erythrose-4-phosphate	199	97	Negative
Xanthurenic acid	204.001	160	Negative
lipoate	205	171	Negative
L-Tryptophan	205	117	Negative
D-glucarate	209	85	Negative
deoxyribose-phosphate	213	79	Negative
L-Zeatine	218	173	Negative
pantothenate	218	146	Negative
prephenate	225	91	Negative

deoxyuridine	227	184	Negative
ribose-phosphate	229	79	Negative
trans, trans-farnesyl diphosphate	381	79	Negative
Indoxyl sulfate	212.0008	212.0008	Negative
1,2-Diethylhydrazine	89.0262	89.0262	Negative
D-Fructose 6-phosphate	303.9778	303.9778	Negative
4-Nitroquinoline-1-oxide	89.0261	89.0261	Negative
Glucoheptonic acid	129.0555	129.0555	Negative
cis-Vaccenic acid	299.9848	299.9848	Negative
2-Butenedioic acid, 2-methyl-, (E)	113.0246	113.0246	Negative
8-Chlorotheophylline	129.0552	129.0552	Negative
6,7-Dimethyltetrahydropterin	197.0682	197.0682	Negative
Flurandrenolide	436.4848	436.4848	Negative
Mevalonic acid	153.0204	153.0204	Negative
3-Cyano-7-ethoxycoumarin	215.0319	215.0319	Negative
4-Nitro-1,3-benzenediamine	154.0614	154.0614	Negative
7,8,4'-Trihydroxyflavone	215.0318	215.0318	Negative
6-Methyluracil	127.0507	127.0507	Negative
Unoprostone	328.4812	328.4812	Negative
DL-Homocysteine, S-ethyl-	148.043	148.043	Negative
N-(4-Nitro-2-phenoxyphenyl)me	308.132	308.132	Negative
Vinburnine	296.1004	296.1004	Negative
Hydroquinine	308.0965	308.0965	Negative
Ursodeoxycholic acid	356.9842	356.9842	Negative
4-Hydroxypropranolol	277.1786	277.1786	Negative
1,3-Dihydrobenzimidazol-2-one	135.0304	135.0304	Negative
Dodecyl sulfate	265.1475	265.1475	Negative
Isobutyric acid	89.0263	89.0263	Negative
5-Sulfosalicylic acid	172.9908	172.9908	Negative
4,6-Dihydroxypyrimidine	129.0562	129.0562	Negative
5-Methylcytosine	127.0501	127.0501	Negative
Monoarachidin	369.1705	369.1705	Negative
3-Cyano-4-ethyl-6-methylcouma	215.0329	215.0329	Negative
D-Glucosaminic acid	114.0553	114.0553	Negative
Triamcinolone	339.1941	339.1941	Negative
Lomefloxacin	352.9856	352.9856	Negative
2-Acetoxy palmitic acid, 2-(N,N,N	401.1295	401.1295	Negative
5,4'-Dihydroxyflavone	255.2334	255.2334	Negative
2,4-O-Ethylidene-D-erythrose	129.0553	129.0553	Negative
Tetrapropylammonium cation	114.0559	114.0559	Negative
2',5'-Dimethoxy-6-fluoroflavone	301.9836	301.9836	Negative
Thymidine 5'-monophosphate	277.033	277.033	Negative
Acenocoumarol	354.9852	354.9852	Negative
Lactacystin	358.9781	358.9781	Negative
5-Azacytosine	114.0557	114.0557	Negative
2,3-Dinor fluprostenol	179.0555	179.0555	Negative
2-Aminoethylphosphonic acid	127.0504	127.0504	Negative

Glycan Man1F	330.4792	330.4792	Negative
14,15-Epoxy-5Z,8Z,11Z-eicosatri	301.9805	301.9805	Negative
Sulfaguanidine	215.0312	215.0312	Negative
Thioguanine	168.0762	168.0762	Negative
Eseroline	220.1193	220.1193	Negative
Carbetapentane	217.0287	217.0287	Negative
Hexadecylmethylglycerol	89.0238	89.0238	Negative
13,14-Dihydro-15(R)-prostagland	354.9842	354.9842	Negative
Tetrahydropalmatine	354.9821	354.9821	Negative
2-Phosphonobutyric acid	335.0464	335.0464	Negative
Chlorsulfuron	358.9783	358.9783	Negative
2-Methylvaleric acid	89.0258	89.0258	Negative
5(S)-HETE	301.9808	301.9808	Negative
DL-3,4-Dihydroxyphenyl glycol	168.0759	168.0759	Negative

**Supplementary Table 1.** List of metabolites with MRM transitions in ESI positive and negative ionization modes.