

Quantitative analysis of endogenous molecules and their metabolites and conjugates by Liquid Chromatography- Hybrid High Resolution Mass Spectrometry (LC-QTOF-5600 Triple TOF)

Table 1: Quantitative analysis of endogenous molecules and their metabolites and conjugates by Liquid Chromatography- Hybrid High Resolution Mass Spectrometry (LC-QTOF-5600 Triple TOF)

S. No.	Amino Acids (AA)	24	L-Homocysteic acid
1	Glutaric acid	25	L-Kynurenine
2	Glycine	26	N-Acetyl-Aspartic acid
3	L-arginine	27	N-Acetyl-L-alanine
4	L-Aspartic acid	28	N-Acetyl-L-phenylalanine
5	L-Glutamine	29	N-Acetylneuraminic acid
6	L-Histidine	30	N-Methyl-L-lysine
7	L-Isoleucine	31	N-Methyl-L-proline
8	L-Leucine	32	NN-Dimethyl Arginine
9	L-Lysine	33	Norepinephrine
10	L-Methionine	34	Phenylacetyl-L-glutamine
11	L-Phenylalanine	35	Pyroglutamic acid
12	L-Proline	36	Sarcosine
13	L-Serine	37	Serotonin
14	L-Tryptophan	38	Stachydrine
15	L-Tyrosine	39	Taurine
		40	Urea
S. No.	AA Metabolites and Conjugates		
1	1-Methyl-L-histidine	S. No.	Carnitine conjugates
2	2-Methyl-N-(4-Methylphenyl)alanine	1	Acetyl-L-carnitine
3	3-Methylindole	2	Butyrylcarnitine
4	3-Methyl-L-histidine	3	Decanoyl-L-carnitine
5	4-Aminohippuric acid	4	Isovalerylcarnitine
6	5-Hydroxylysine	5	Lauroyl-L-carnitine
7	5-Hydroxymethyluracil	6	L-Glutarylcarnitine
8	Alpha-Aspartyl-lysine	7	Linoleoylcarnitine
9	Argininosuccinic acid	8	L-Propionylcarnitine
10	Betaine	9	Myristoyl-L-carnitine
11	Betonicine	10	Octanoylcarnitine
12	Carnitine	11	Oleoyl-L-carnitine
13	Creatine	12	Palmitoyl-L-carnitine
14	Creatinine	13	Stearoyl-L-carnitine
15	Dimethylglycine		
16	Dopamine	S. No.	Krebs Cycle
17	Epinephrine	1	Aconitate
18	Hippuric acid	2	Citrate
19	Homo-L-arginine	3	Ketoglutarate
20	Hydroxykynurenine	4	Malate
21	Indolelactic acid	5	Oxalo acetate
22	L-Alloisoleucine	6	Succinate
23	L-Citrulline		
24	L-Cysteine-glutathione disulfide		
25	L-Glutathione, reduced		

Quantitative analysis of endogenous molecules and their metabolites and conjugates by Liquid Chromatography- Hybrid High Resolution Mass Spectrometry (LC-QTOF-5600 Triple TOF)

S. No.	Energy Metabolism	S. No.	Vitamin & Cofactor metabolism
1	Adenosine triphosphate	1	Niacinamide
2	Butyrate	2	Pyridoxine
3	Citrate	3	4-Pyridoxic acid
4	D-Ribose 5-phosphate	4	Ascorbic acid
5	Glucose	5	Dehydroascorbic acid
6	Lactic acid	6	Nicotinic acid
7	Oxaloacetate	7	Pyridoxal 5-phosphate
8	Pyruvate	8	Pyridoxamine
		9	Pantothenic acid
S. No.	Nucleic acid Metabolism and conjugates	S. No.	Steroid & Bile Acids Metabolism
1	1-Methyladenosine	1	Cholic acid (CA)
2	1-Methylguanine	2	Chenodeoxycholic acid
3	Adenosine	3	Glycoursodeoxycholic acid
4	Adenosine diphosphate	4	Glycocholic acid
5	Adenylosuccinic acid	5	Glycodeoxycholic acid
6	Cytidine 3'-monophosphate	6	Taurocholic acid
7	Cytidine 5'-diphosphate ethanolamine	7	3-Dehydroepiandrosterone sulfate
8	Cytidine triphosphate	8	(3.beta.)-Allopregnanolone sulfate
9	Guanine	9	5.alpha.-Androstan-3.beta.-ol-17-one sulfate
10	Guanosine	10	4-Androsten-17.beta.-ol-3-one sulfate
11	Guanosine diphosphate	11	(5.alpha.)-2'H-Androst-2-eno3,2-cpyrazol-17-one
12	Hypoxanthine		
13	Inosine	S. No.	Other metabolites and small molecules
14	L-Cysteine-glutathione disulfide	1	(-)-Cotinine
15	Uric acid	2	(+)-trans-Chrysanthemic acid
16	Uridine	3	(3.beta.)-Allopregnanolone sulfate
17	Xanthine	4	1,2-Benzenedicarboxylic acid
		5	13-cis-Retinoic acid
S. No.	Carbohydrates	6	2,2-Dimethylsuccinic acid
1	D-Lyxose	7	2,5-Furandicarboxylic acid
2	Glucose	8	2,6-Dihydroxybenzoic acid
3	Glucose-6-phosphate	9	2-Aminobenzoic acid
4	L-Sorbose	10	2-Aminoisobutyric acid
5	Pyruvate	11	2-Furoylglycine
6	D-Ribose	12	2-Hydroxybutyric acid
7	Threonic acid	13	2-Hydroxycaproic acid

Quantitative analysis of endogenous molecules and their metabolites and conjugates by Liquid Chromatography- Hybrid High Resolution Mass Spectrometry (LC-QTOF-5600 Triple TOF)

S. No.	Other metabolites and small molecules	52	Glycerol 3-phosphate
14	2-Hydroxyoctanoic acid	53	Glycerophosphocholine
15	2-Ketobutyric acid	54	Hexamethylenetetramine
16	2-Phenylbutyric acid	55	Imidazoleacetic acid
17	2-Piperidinone	56	Indoxyl sulfate
18	3-(2-Hydroxyphenyl)propionic acid	57	Ingenol
19	3-Aminopentanoic acid	58	Kaempferol
20	3-Hexenedioic acid	59	m-Cresol
21	3-Hydroxybenzaldehyde	60	Metoprolol
22	3-Hydroxybenzoic acid	61	Metoprolol acid
23	3-Hydroxybutyric acid	62	Monastrol
24	3-Hydroxydodecanoic acid	63	N-(tert-Butyl)benzenesulfonamide
25	3-Methoxytyramine	64	Norquetiapine
26	3-Methyladipic acid	65	N-Propylamphetamine
27	3-Methylcrotonic acid	66	p-Acetamidophenyl -glucuronide
28	3-Methylphenylacetic acid	67	Paraxanthine
29	4-Guanidinobutanoic acid	68	PyroGlu-Ile-Arg
30	4-Hydrazinobenzenesulfonic acid	69	Quetiapine sulfoxide
31	4-Hydroxybenzoic acid	70	Tetrahydroharmine
32	4-Methylacetophenone	71	Theobromine
33	4-Pyridoxic acid		
34	5-Amino-1-pentanol	S. No.	Fatty acids and derivatives
35	5-Aminovaleric acid	1	2-cis-Hexadecenoic acid
36	5-Hydroxyindole	2	2-Hydroxypalmitic acid
37	5-Phenylvaleric acid	3	5,6-Dehydroarachidonic acid
38	6-Amino-1-hexanol	4	Arachidonic acid
39	Acetaminophen	5	Azelaic acid
40	Acetaminophen sulfate	6	Butanoic acid
41	Alpha-ketoisovaleric acid	7	Elaidic acid
42	Aminobutyrate	8	Decanoic acid
43	Benzenesulfonic acid	9	DELTA.2-cis-Hexadecenoic acid
44	Butyrolactone	10	Dodecanedioic acid
45	Caffeine	11	Hexadecanedioic acid
46	Cholesterol 3-sulfate	12	Linoleic acid
47	D-Glucurono-6,3-lactone	13	Myristoleic acid
48	DL-2-Amino-octanoic acid	14	O-Arachidonoylglycidol
49	Dodecyl sulfate	15	Oleic acid
50	Dodecylbenzenesulfonic acid	16	Palmitic acid
51	Gabapentin	17	Undecanedioic acid

Quantitative analysis of endogenous molecules and their metabolites and conjugates by Liquid Chromatography- Hybrid High Resolution Mass Spectrometry (LC-QTOF-5600 Triple TOF)

S. No.	Fatty acids and derivatives
18	8,11-Tridecadienoic acid, 13-(3-pentyl-2-oxiranyl)
19	9-Oxo-10(E),12(E)-octadecadienoic acid
20	cis-4,10,13,16-Docosatetraenoic acid
21	cis-4,7,10,13,16,19-Docosahexaenoic acid
22	8,11-Eicosadiynoic acid
23	Cis-8,11,14-Eicosatrienoic acid
24	Cis-5,8,11,14-Eicosatetraenoic acid
25	Cis-5,8,11,14-Eicosatetraenoic acid, 16-hydroxy
26	8(9)-Epoxy-5Z,11Z,14Z-eicosatrienoic acid
28	13-Hydroxy-9Z,11E-octadecadienoic acid
29	16-Hydroxy-4Z,7Z,10Z,13Z,17E,19Z-docosahexaenoic acid
30	19(20)-Epoxy-4Z,7Z,10Z,13Z,16Z-docosapentaenoic acid
31	Sebacic acid
32	Stearic acid
S. No.	Lipids
1	1-Palmitoylglycerol
1	1-(1Z-Hexadecenyl)-sn-glycero-3-phosphocholine
2	1-(1Z-Octadecenyl)-2-(5Z,8Z,11Z,14Z-eicosatetraenoyl)-sn-glycero-3-phosphocholine
3	1-(1Z-Octadecenyl)-sn-glycero-3-phosphocholine
4	1,2-dioleoyl-sn-glycero-3-phosphatidylcholine
5	1,2-Dioleoyl-sn-glycero-3-phosphoethanolamine
6	1-Heptadecanoyl-sn-glycero-3-phosphocholine
7	1-Hexadecyl-2-(5Z,8Z,11Z,14Z-eicosatetraenoyl)-sn-glycero-3-phosphocholine
8	1-Hexadecyl-sn-glycero-3-phosphocholine
9	1-Octadecyl-2-acetyl-sn-glycero-3-phosphocholine
10	1-O-Hexadecyl-2-O-(2E-butenoyl)-sn-glyceryl-3-phosphocholine
11	1-O-Hexadecyl-2-O-acetyl-sn-glyceryl-3-phosphorylcholine
12	1-Oleoyl-2-myristoyl-sn-glycero-3-phosphocholine
13	1-Oleoyl-sn-glycero-3-phosphocholine
14	1-Oleoyl-sn-glycero-3-phosphoethanolamine
15	1-Palmitoyl-2-arachidonoyl-sn-glycero-3-phosphocholine
16	1-Palmitoyl-2-docosahexaenoyl-sn-glycero-3-phosphocholine
17	1-Palmitoyl-2-hydroxy-sn-glycero-3-phosphoethanolamine
19	1-Palmitoyl-2-linoleoyl-sn-glycero-3-phosphocholine
20	1-Palmitoyl-sn-glycero-3-phosphocholine
21	1-Stearoyl-2-docosahexaenoyl-sn-glycero-3-phosphocholine
22	1-Stearoyl-2-hydroxy-sn-glycero-3-phosphocholine
23	1-Stearoyl-2-hydroxy-sn-glycero-3-phosphoethanolamine
25	2-(5-Oxovaleryl)phosphatidylcholine
26	2-Oleoyl-1-palmitoyl-sn-glycero-3-phosphocholine