

**Supplementary Table 1: KEGG pathway for identified biomarkers**

Biomarker	KEGG number	Primary Biological pathway/ function
1-Linoleoylglycerol (1-monolinolein)	-	Cell signaling, energy source and storage, membrane integrity/stability
1-Monopalmitin	-	Cell signaling, energy source and storage, membrane integrity/stability
1-Palmitoylglycerophosphoinositol		Glycerophosphoinositols
11-HETE	C14780	Arachidonic acid metabolism
12-HETE	-	Arachidonic acid metabolism
12-HHTrE	-	Arachidonic acid metabolism
12-Ketodeoxycholic acid	-	Bile acid
14,15-DiHETE	-	Arachidonic acid metabolism
14,15-DiHETrE	-	Arachidonic acid metabolism
17,18-DiHETE	-	Eicosapentaenoic acid metabolism
2-Hydroxyglutarate	C02630	Butanoate metabolism; C5-branched dibasic acid metabolism
2-Hydroxypalmitic acid	-	Cell signaling, energy source and storage, membrane integrity/stability
2-Ketobutyric acid	C00109	Amino acid metabolism (glycine, methionine, valine, leucine etc); C5-branched dibasic acid metabolism
2-Monostearin	-	-
2-Oxoglutarate (alpha-ketoglutarate)	C00026	TCA cycle
2'-Deoxycytidine	C00881	Pyrimidine metabolism
2'-Deoxyuridine	C00526	Pyrimidine metabolism
2'-Deoxyxanthosine	-	Purine metabolism
3-Hydroxy-2-methylbenzoic acid <i>O</i> -sulfate	-	-
3-Hydroxybutanoate	C01089	Synthesis and degradation of ketone bodies; Butanoate metabolism; cAMP signaling pathway
3-Hydroxyoleoylcarnitine C18:1-OH	-	Acylcarnitine, fatty acid $\beta$ -oxidation
3-hydroxytyrosol sulfate		Tyrosols
3-Indoxyl sulfate	-	Tryptophan metabolism
3-Oxo-octadecanoic acid	-	Fatty acid biosynthesis
4-Aminobutanoate	C00334	Alanine, aspartate, butanoate, glutamate, taurine and hypotaurine metabolism
4-Guanidinobutanoic acid	C01035	Arginine and proline metabolism
4-Hydroxyphenylpyruvic acid	C01179	Biosynthesis of amino acids; 2-oxocarboxylic acid metabolism
4-Pyridoxic acid	C00847	Vitamin B6 metabolism
5-Hydroxy-L-tryptophan	C01017	Tryptophan metabolism
5,6-Dihydrouracil	C00429	Pyrimidine metabolism
7-Sulfocholic acid	-	Dihydroxy bile acids, alcohols, and derivatives
8-HETE	C14776	Arachidonic acid metabolism
9-HOTrE	-	$\alpha$ -linolenic acid metabolism
Acetylcarnitine	C02571	Acylcarnitine, fatty acid $\beta$ -oxidation
Acetylornithine	C00437	Arginine biosynthesis; 2-oxocarboxylic acid metabolism
Adipic acid	C00322	Lysine, tryptophan, methane metabolism; 2-oxocarboxylic acid metabolism
Adrenic acid	C16527	Biosynthesis of unsaturated fatty acids
Alanine	C00041	Alanine, aspartate, glutamate, cysteine, methionine metabolism; Taurine and hypotaurine metabolism
Allantoin	C01551	Purine metabolism
Linoleic acid	C01595	Linoleic acid metabolism
Arabinonate	C00545	Ascorbate and aldarate metabolism
Arabitol	C00532	Pentose and glucuronate metabolism
Arachidonic acid	C00219	Arachidonic acid metabolism
Arginine	C00062	Arginine and ornithine metabolism; Aminoacyl t-RNA biosynthesis
Asparagine	C00152	Alanine, aspartate, glutamate metabolism
Aspartic acid	C00049	Various amino acid metabolism pathways; Aminoacyl t-RNA biosynthesis
Azelaic acid	C08261	Medium chain fatty acids
Benzoic acid	C00180	Phenylalanine metabolism; Benzoate metabolism
beta-Alanine	C00099	Pyrimidine metabolism; beta-alanine metabolism; propanoate metabolism
Betaine	C00719	Glycine, serine, and threonine metabolism
Butyrylcarnitine	C02862	Acylcarnitine, fatty acid $\beta$ -oxidation
Carnitine	C00318	Fatty acid $\beta$ -oxidation
Chenodeoxycholic acid sulfate	-	Monohydroxy bile acids, alcohols, and derivatives
ChoE(18:1)	-	Cholesteryl ester
ChoE(18:2)	-	Cholesteryl ester
ChoE(20:4)	-	Cholesteryl ester
ChoE(20:4)	-	Cholesteryl ester
ChoE(22:6)	-	Cholesteryl ester
Choline	C00114	Glycine, serine and threonine metabolism; Glycerophospholipid metabolism; Bile secretion
Cinnamoylglycine	-	Excreted plant product
<i>cis</i> -Aconitic acid	C00417	TCA cycle

<i>cis</i> -OH Proline	C01015	Hydroxylated proline
Citrate (citric acid)	C00158	TCA cycle
Citrulline	C00327	Arginine biosynthesis, urea cycle
Cortisol	C00735	Steroid hormone biosynthesis
Cortisone	C00762	Steroid hormone biosynthesis
Creatine	C00300	Glycine, serine, and threonine metabolism; Arginine and proline metabolism
Creatinine	C00791	Arginine and proline metabolism
Cysteine	C00097	Glycine, serine, and threonine metabolism; Cysteine and methionine metabolism
Cystine	C00491	Cysteine and methionine metabolism; ABC transporters
Cytosine	C00380	Pyrimidine metabolism
dAMP	C00360	Purine metabolism
Decanoylcarnitine	-	Acylcarnitine, fatty acid $\beta$ -oxidation
DG (34:1)	-	Diacylglycerol
DG (34:2)	-	Diacylglycerol
DG (36:1)	-	Diacylglycerol
DG (36:2)	-	Diacylglycerol
DG (36:3)	-	Diacylglycerol
DG (36:4)	-	Diacylglycerol
DG (44:12)	-	Diacylglycerol
DG(39:3)	-	Diacylglycerol
DG(43:3)	-	Diacylglycerol
Dihydroliipoamide	C00579	Glycolysis/ gluconeogenesis; TCA cycle; Alanine, aspartate, pyruvate metabolism; Valine, Leucine and Isoleucine metabolism
Dimethylglycine	C01026	Glycine, serine, and threonine metabolism
Dityrosine	-	Amino acid biosynthesis
Docosahexaenoic acid	C06429	Biosynthesis of unsaturated fatty acids
Dodecanedioic acid	C02678	Fatty acid $\beta$ -oxidation
Eicosapentanoate (EPA; 20:5n3)	C06428	Eicosapentaenoic acid metabolism (precursor)
ePC (24:0)	-	Ether linked phosphatidylcholine
ePC (30:0)	-	Ether linked phosphatidylcholine
ePC (32:2)	-	Ether linked phosphatidylcholine
ePC (34:2)	-	Ether linked phosphatidylcholine
ePC (34:4)	-	Ether linked phosphatidylcholine
ePC (36:1)	-	Ether linked phosphatidylcholine
ePC (36:2)	-	Ether linked phosphatidylcholine
ePC (36:5)	-	Ether linked phosphatidylcholine
ePC (40:6)	-	Ether linked phosphatidylcholine
ePC (42:4)	-	Ether linked phosphatidylcholine
ePE (34:3)	-	Ether linked phosphatidylcholine
ePE (36:2)	-	Ether linked phosphatidylcholine
ePE (36:3)	-	Ether linked phosphatidylcholine
ePE (36:4)	-	Ether linked phosphatidylcholine
ePE (38:5)	-	Ether linked phosphatidylcholine
ePE (38:6)	-	Ether linked phosphatidylcholine
ePE (38:7)	-	Ether linked phosphatidylcholine
ePE (40:5)	-	Ether linked phosphatidylcholine
ePE (40:7)	-	Ether linked phosphatidylcholine
ePE (40:8)	-	Ether linked phosphatidylcholine
Equol sulfate	C14131 for equol	Isoflavanol
Ferulic acid	C01494	Phenylpropanoid biosynthesis
Flavin mononucleotide	C00061	Oxidative phosphorylation; Riboflavin metabolism
Fructose	C00095	Fructose and mannose metabolism
Fucose	C01019	Fructose and mannose metabolism; Amino acid and nucleotide sugar metabolism
Fumarate/ Fumaric acid	C00122	TCA cycle
Gentisic acid	C00628	Tyrosine metabolism
Glucarate	C00818	Ascorbate and aldarate metabolism
Gluconic acid	C00257	Pentose phosphate pathway
Glucose	C00031	Glycolysis/ Gluconeogenesis; Pentose phosphate pathway; Amino acid and nucleotide sugar metabolism
Glucuronic acid	C00191	Pentose and glucuronate interconversions; Ascorbate and aldarate metabolism
Glutaconic acid	C02214	Cell signaling, energy source and storage, membrane integrity/stability
Glutamate/ Glutamic acid	C00025	Various amino acid metabolism; Glutathione metabolism; C5-branched chain amino acid metabolism
Glutamine	C00064	Arginine, alanine, aspartate, glutamate metabolism; Purine and pyrimidine metabolism
Glyceric acid	C00258	Pentose phosphate pathway; Glycine, serine, threonine metabolism; Glycerolipid metabolism

Glycerol	C00116	Pentose and glucuronate interconversions; Glycerolipid metabolism; Galactose metabolism
Glycerol-3-phosphate	C00093	Glycerolipid metabolism; Glycerophospholipid metabolism
Glycine	C00037	Bile acid biosynthesis; Purine metabolism; Glycine, serine, threonine, lysine, thiamine, glutathione metabolism
Glycolic acid	C00160	Glyoxylate and dicarboxylate metabolism
Glyoxylic acid	C00048	Purine metabolism; Glycine, serine, threonine, arginine, proline, methane metabolism
Gulonolactone	C01040	Ascorbate and aldarate metabolism
Heme	C00032	Porphyrin and chlorophyll metabolism
Hexanoylcarnitine	-	Acylcarnitine, fatty acid $\beta$ -oxidation
Hexanoylglycine	-	Fatty acid $\beta$ -oxidation
Hippurate (Hippuric acid)	C01586	Phenylalanine metabolism
Histidine	C00135	Histidine, beta-alanine metabolism; Aminoacyl t-RNA biosynthesis
Homogentisic acid	C00544	Ubiquinone biosynthesis; Tyrosine metabolism
Homotachydrine	C08283	Alkaloid derived from ornithine, phytochemical
Hydroquinone	C00530	Tyrosine metabolism; Riboflavin metabolism
Hypoxanthine	C00262	Purine metabolism
Indole-3-acetamide	C02693	Tryptophan metabolism
Indole-3-carboxylic acid	C19837	Tryptophan metabolism
Indole-3-pyruvate	C00331	Tryptophan metabolism
Indoleacetic acid	C00954	Tryptophan metabolism
Indolelactate	C02043	Tryptophan metabolism
Indolepropionate	-	Tryptophan metabolism
Inositol	C00137	Galactose metabolism; Ascorbate and aldarate metabolism; Inositol phosphate metabolism
Isovalerylglycine	-	Fatty acid $\beta$ -oxidation
Isethionic acid	C05123	Taurine and hypotaurine metabolism
Isobutyryl-L-carnitine/butyrylcarnitine	-	Acylcarnitine, fatty acid $\beta$ -oxidation
Isocitrate	C00311	TCA cycle
Isoleucine/Leucine	C00407/ C00123	Valine, leucine, isoleucine metabolism; Aminoacyl t-RNA biosynthesis
Kynurenic acid	C01717	Tryptophan metabolism
L-Alloisoleucine	-	Isoleucine transamination