

Metabolite	CAS	KEGG
3-hydroxybutyric acid	300-85-6	C01089
5-Hydroxylysine		
Acetyl CoA		C00024
N-Acetyl-L-aspartic acid	997-55-7	
acetyl-carnitine	3040-38-8	C02571
Acetylcholine	51-84-3	C01996
Acetylcysteine	616-91-1	C06809
N-Acetylglutamine		
N6-Acetyl-L-lysine		
Adenine	73-24-5	C00147
Adenosine	58-61-7	C00212
ADP	58-64-0	C00008
alpha-Ketoglutaric acid	328-50-7	C00026
Amino adipate	542-32-5	C00956
AMP	61-19-8	C00020
Arachidonic acid	506-32-1	C00219
Arginine	74-79-3	C00062
Argininosuccinate	2387-71-5	C03406
Asparagine	70-47-3	C00152
Aspartate	56-84-8	C00049
ATP	56-65-5	C00002
beta Alanine	107-95-9	C00099
Betaine	107-43-7	C00719
Butyric acid	107-92-6	C00246
Butyrylcarnitine		C02862
Caprylic acid	124-07-2	C06423
Carnitine	541-15-1	C00318
Carnosine	305-84-0	C00386
CDP	63-38-7	C00112
Choline	62-49-7	C00114
cis-aconitate	585-84-2	C00417
Citrate	77-92-9	C00158
Citrulline	372-75-8	C00327
CMP	63-37-6	C00055
Coenzyme A	85-61-0	C00010
Creatine	57-00-1	C00300
Creatinine	60-27-5	C00791
CTP	65-47-4	C00063
Cystathionine	56-88-2	C02291
Cystine	56-89-3	C00491
Cytidine	65-46-3	C00475
Decanoic acid	172,2646	C01571
Decanoylcarnitine	1492-27-9	
Dihydroxyacetone phosphate	57-04-5	C00111
Docosaehaenoic acid	6217-54-5	C06429
dodecanoic acid	143-07-7	C02679
Dodecanoylcarnitine	25518-54-1	
Eicosapentaenoic acid	10417-94-4	
ethanolamine phosphate	1071-23-4	C00346
FAD	146-14-5	C00016

Folate	59-30-3	C00504
fructose 1,6-diphosphate	488-69-7	C00354
Fumarate	110-17-8	C00122
GDP	146-91-8	C00035
Glutamine	56-85-9	C00064
Glutamate	6893-26-1	C00217
Glucose	50-99-7	C00031
Glucose-6-phosphate	56-73-5	C00092
D-Glyceraldehyde 3-phosphate	142-10-9	C00661
Glycerol 3-phosphate	57-03-4	C00093
Glycine	56-40-6	C00037
GMP	85-32-5	C00144
GSH	70-18-8	C00051
GSSG	27025-41-8	C00127
GTP	86-01-1	C00044
Guanine	73-40-5	C00242
Guanosine	118-00-3	C00387
Hexanoic acid	142-62-1	C01585
Hexanoyl-L-carnitine	6418-78-6	
Histidine	71-00-1	C00135
Homocysteine	6027-13-0	C00155
Hydroxy-L-proline	51-35-4	C01157
Hypoxanthine	68-94-0	C00262
IMP	131-99-7	C00130
Inosine	58-63-9	C00294
IsoLeucine	73-32-5	C00407
Lactate	79-33-4	C00186
L-Alanine	56-41-7	C00041
L-alpha-Amino-N-butyric acid	1492-24-6	C02356
L-beta-Aminoisobutyric acid	4249-19-8	C03284
Leucine	61-90-5	C00123
Linoleic acid	60-33-3	C01595
Linolenic acid	463-40-1	C06427
L-Sarcosine	107-97-1	C00213
Lysine	56-87-1	C00047
Malate	97-67-6	C00149
Methionine	63-68-3	C00073
N(6)-Methyllysine	1188-07-4	C02728
1-Methylhistidine	368-16-1	C01152
Myristic acid	544-63-8	C06424
Myristoylcarnitine	25597-07-3	
NAD+	53-84-9	C00003
NADH	58-68-4	C00004
NADP+	53-59-8	C00006
NADPH	53-57-6	C00005
Nicotinate	59-67-6	C00253
Nicotinamide	98-92-0	C00153
Nicotinamide N-oxide	1986-81-8	
L-Octanoylcarnitine	25243-95-2	C02838
Oleic acid	112-80-1	C00712
O-Phosphoethanolamine	1071-23-4	C00346
O-Phospho-L-serine	17885-08-4	C01005

Ornithine	70-26-8	C00077
Oxoadipate	3184-35-8	C00322
Oxypurinol	2465-59-0	C07599
Palmitic acid	57-10-3	C00249
Palmitoleic acid	373-49-9	C08362
Palmitoylcarnitine	2364-67-2	C02990
Pantothenate	79-83-4	C00864
2-phosphoenolpyruvate	138-08-9	C00074
Phenol red	143-74-8	
Phenylalanine	63-91-2	C00079
Phosphocreatine	67-07-2	C02305
picolinate		
Proline	147-85-3	C00148
Propionyl-carnitine	17298-37-2	C03017
pyridoxal		
Pyruvate	127-17-3	C00022
Riboflavin	83-88-5	C00255
Ribose	50-69-1	C00121
Ribose 1-phosphate	14075-00-4	C00620
S-Adenosyl-L-Homocysteine	979-92-0	C00021
S-Adenosyl-L-methionine	29908-03-0	C00019
D-Sedoheptulose 7-phosphate	2646-35-7	C05382
Serine	56-45-1	C00065
Stearic acid	57-11-4	C01530
Succinic acid	110-15-6	C00042
S-Cysteinossuccinic acid		
S-succinylglutathione		
Taurine	107-35-7	C00245
Thiamine		
Threonine	72-19-5	C00188
Thymidine		
Tryptophan	73-22-3	C00078
Tyrosine	60-18-4	C00082
UDP	58-98-0	C00015
UDP-GlcNAc	528-04-1	C00043
UMP	58-97-9	C00105
Urate	69-93-2	C00366
Uridine	58-96-8	C00299
Uridine diphosphate glucose	133-89-1	C00029
UTP	63-39-8	C00075
Valine	72-18-4	C00183
Xanthine	69-89-6	C00385
Xanthosine		
Xanthylic acid		