

Metabolite name	Chemical formula	KEGG/HMDB/ PubChem Identifier
glyoxylate	C2H2O3	C00048
glycolate	C2H4O3	C00160
pyruvate	C3H4O3	C00022
lactate	C3H6O3	C00186
2-oxobutanoate	C4H6O3	C00109
acetoacetate	C4H6O3	C00164
glycerate	C3H6O4	C00258
uracil	C4H4N2O2	C00106
fumarate	C4H4O4	C00122
Maleic acid	C4H4O4	C01384
2-keto-isovalerate	C5H8O3	C00141
Guanidoacetic acid	C3H7N3O2	C00581
succinate	C4H6O4	C00042
Methylmalonic acid	C4H6O4	C02170
3-S-methylthiopropionate	C4H8O2S	C08276
nicotinate	C6H5NO2	C00253
taurine	C2H7NO3S	C00245
Pyroglutamic acid	C5H7NO3	C01879
Citraconic acid	C5H6O4	C02226
2-ketohexanoic acid	C6H10O3	HMDB01864
N-Acetyl-L-alanine	C5H9NO3	C01073
oxaloacetate	C4H4O5	C00036
Hydroxyisocaproic acid	C6H12O3	HMDB00746
malate	C4H6O5	C00149
hypoxanthine	C5H4N4O	C00262
anthranilate	C7H7NO2	C00108
p-aminobenzoate	C7H7NO2	C00568
p-hydroxybenzoate	C7H6O3	C00156
acetylphosphate	C2H5O5P	C00227
Carbamoyl phosphate	CH4NO5P	C00169
a-ketoglutarate	C5H6O5	C00026
Phenylpropionic acid	C9H6O2	HMDB00563
2-oxo-4-methylthiobutanoate	C5H8O3S	C01180
2-Hydroxy-2-methylbutanedioic acid	C5H8O5	C02612
3-methylphenylacetic acid	C9H10O2	HMDB02222
xanthine	C5H4N4O2	C00385
Hydroxyphenylacetic acid	C8H8O3	C05852
2,3-dihydroxybenzoic acid	C7H6O4	C00196
orotate	C5H4N2O4	C00295
dihydroorotate	C5H6N2O4	C00337
allantoin	C4H6N4O3	C01551
Amino adipic acid	C6H11NO4	C00956
Indole-3-carboxylic acid	C9H7NO2	HMDB03320
phenylpyruvate	C9H8O3	C00166
Atrolactic acid	C9H10O3	HMDB00475
Phenyllactic acid	C9H10O3	C01479
quinolinate	C7H5NO4	C03722
phosphoenolpyruvate	C3H5O6P	C00074
Uric acid	C5H4N4O3	C00366
dihydroxy-acetone-phosphate	C3H7O6P	C00111

D-glyceraldehyde-3-phosphate	C3H7O6P	C00111
sn-glycerol-3-phosphate	C3H9O6P	C00093
shikimate	C7H10O5	C04236
aconitate	C6H6O6	C00417
allantoate	C4H8N4O4	C00499
Ascorbic acid	C6H8O6	C00072
2-Isopropylmalic acid	C7H12O5	C02504
N-carbamoyl-L-aspartate_neg	C5H8N2O5	C00438
Pyrophosphate	P2H4O7	C00013
glucono-D-lactone	C6H10O6	C00198
myo-inositol	C6H12O6	C00137
hydroxyphenylpyruvate	C9H8O4	C01179
homocysteic acid	C4H9NO5S	C16511
4-Pyridoxic acid	C8H9NO4	C00847
3-phosphoglycerate	C3H7O7P	C00197
Indoleacrylic acid	C11H9NO2	HMDB00734
Kynurenic acid	C10H7NO3	C01717
citrate-isocitrate	C6H8O7	C00158
isocitrate	C6H8O7	C00311
citrate	C6H8O7	C00158
2-dehydro-D-gluconate	C6H10O7	C00629
D-gluconate	C6H12O7	C00257
D-erythrose-4-phosphate	C4H9O7P	C00279
Xanthurenic acid	C10H7NO4	C02470
lipoate	C8H14O2S2	C00725
D-glucarate	C6H10O8	C00767
deoxyribose-phosphate	C5H11O7P	C00673
pantothenate	C9H17NO5	C00864
prephenate	C10H10O6	C00251
deoxyuridine	C9H12N2O5	C00526
ribose-phosphate	C5H11O8P	C00117
thymidine	C10H14N2O5	C00214
uridine	C9H12N2O6	C00299
deoxyinosine	C10H12N4O5	C05512
shikimate-3-phosphate	C7H11O8P	C03175
6-phospho-D-glucono-1,5-lactone	C6H11O9P	C01236
hexose-phosphate	C6H13O9P	C00085
glucose-1-phosphate	C6H13O9P	C00103
glucose-6-phosphate	C6H13O9P	C00085
fructose-6-phosphate	C6H13O9P	C00085
1,3-diphosphoglycerate	C3H8O10P2	C00236
2,3-Diphosphoglyceric acid	C3H8O10P2	C01159
S-ribosyl-L-homocysteine_neg	C9H17NO6S	C03539
inosine	C10H12N4O5	C00294
6-phospho-D-gluconate	C6H13O10P	C00345
xanthosine	C10H12N4O6	C01762
D-sedoheptulose-1-7-phosphate	C7H15O10P	C05382
N-acetyl-glucosamine-1-phosphate	C6H14NO8P	C03783
glutathione_neg	C10H17N3O6S	C00051
dUMP_neg	C9H13N2O8P	C00365
Geranyl-PP	C10H20O7P2	C00341
octulose-monophosphate (O8P-O1P)	C8H17O11P	

dTMP_neg	C10H15N2O8P	C00364
cyclic-AMP	C10H12N5O6P	C00575
fructose-1,6-bisphosphate	C6H14O12P2	C00354
trehalose-sucrose	C12H22O11	C00089
Cellobiose	C12H22O11	C00185
orotidine-5-phosphate	C10H13N2O11P	C01103
Sedoheptulose 1,7-bisphosphate (SBP)	C7H16O13P2	C00447
trans, trans-farnesyl diphosphate	C15H28O7P2	C00448
S-adenosyl-L-homocysteine_neg	C14H20N6O5S	C00021
dCDP_neg	C9H15N3O10P2	C00705
5-phosphoribosyl-1-pyrophosphate	C5H13O14P3	C00119
Deoxycholic acid	C26H43NO5	C05464
octulose-1,8-bisphosphate (OBP)	C8H18O14P2	
dTDP_neg	C10H16N2O11P2	C00363
CDP_neg	C9H15N3O11P2	C00112
UDP_neg	C9H14N2O12P2	C00015
Cholic acid	C24H40O5	HMDB00619
trehalose-6-Phosphate	C12H23O14P	C00689
Thiamine pyrophosphate	C12H19N4O7P2S	C00068
adenosine 5-phosphosulfate	C10H14N5O10PS	C00224
ADP_neg	C10H15N5O10P2	C00008
dGDP_neg	C10H15N5O10P2	C00008
IDP_neg	C10H14N4O11P2	C00104
GDP_neg	C10H15N5O11P2	C00035
CDP-ethanolamine	C11H20N4O11P2	C00570
FMN	C17H21N4O9P	C00061
cholesteryl sulfate	C27H46O4S	HMDB00653
dCTP_neg	C9H16N3O13P3	C00458
dUTP_neg	C9H15N2O14P3	C00460
dTTP_neg	C10H17N2O14P3	C00459
CTP_neg	C9H16N3O14P3	C00063
UTP_neg	C9H15N2O15P3	C00075
CDP-choline	C14H27N4O11P2	C00307
dATP_neg	C10H16N5O12P3	C00131
Taurodeoxycholic acid	C26H45NO6S	C05463
ATP_neg	C10H16N5O13P3	C00002
dGTP	C10H16N5O13P3	C00002
GTP_neg	C10H16N5O13P3	C00002
UDP-D-glucose	C15H24N2O17P2	C00029
UDP-D-glucuronate	C15H22N2O18P2	C00167
ADP-D-glucose	C16H25N5O15P2	C00498
guanosine 5-diphosphate,3-diphosphate	C10H11N5O17P4	C01228
UDP-N-acetyl-glucosamine	C17H27N3O17P2	C00043
glutathione disulfide_neg	C20H32N6O12S2	C00127
NAD+_neg	C21H27N7O14P2	C00003
NADH_neg	C21H29N7O14P2	C00004
dephospho-CoA_neg	C21H35N7O13P2S	C00882
cyclic bis(3->5) dimeric GMP	C20H24N10O14P2	C16463
NADP+_neg	C21H28N7O17P3	C00006
NADPH_neg	C21H30N7O17P3	C00005
coenzyme A_neg	C21H36N7O16P3S	C00010
acetyl-CoA_neg	C23H38N7O17P3S	C00024

propionyl-CoA_neg	C24H40N7O17P3S	C00100
butyryl-CoA	C25H42N7O17P3S	C00630
acetoacetyl-CoA_neg	C25H40N7O18P3S	C00332
malonyl-CoA_neg	C24H38N7O19P3S	C00083
3-hydroxybutyryl-CoA	C25H42N7O18P3S	C01144
succinyl-CoA-methylmalonyl-CoA_neg	C25H40N7O19P3S	C00091
3-hydroxy-3-methylglutaryl-CoA_neg	C27H44N7O20P3S	C00356
2-deoxyglucose-6-phosphate	C6H13O8P	C06369
2-hydroxygluterate	C5H8O5	C03196

Urea	CH4N2O	C00086
ethanolamine	C2H7NO	C00189
Imidazole	C3H4N2	C01589
glycine	C2H5NO2	C00037
alanine	C3H7NO2	C00041
betaine aldehyde	C5H12NO	C00576
choline	C5H14NO	C00114
4-aminobutyrate	C4H9NO2	C00334
dimethylglycine	C4H9NO2	C01026
serine	C3H7NO3	C00065
cytosine	C4H5N3O	C00380
Creatinine	C4H7N3O	C00791
proline	C5H9NO2	C00148
indole	C8H7N	C16074
betaine	C5H11NO2	C00719
valine	C5H11NO2	C00183
threonine	C4H9NO3	C00188
homoserine	C4H9NO3	C00263
purine	C5H4N4	C00465
cysteine	C6H12N2O4S2	C00491
creatine	C4H9N3O2	C00300
nicotinamide	C6H6N2O	C00153
Imidazoleacetic acid	C6H8N2O2	C05828
thymine	C5H6N2O2	C00178
DL-Pipecolic acid	C6H11NO2	C00408
N-Acetylputrescine	C6H14N2O	C02714
hydroxyproline	C5H9NO3	C01157
leucine-isoleucine	C6H13NO2	C00123
ornithine	C5H12N2O2	C00077
asparagine	C4H8N2O3	C00152
aspartate	C4H7NO4	C00049
adenine	C5H5N5	C00147
Methylcysteine	C4H9NO2S	C00155
homocysteine	C4H9NO2S	C00155
methylnicotinamide	C7H9N2O	C02918
histidinol	C6H11N3O	C00860
lysine	C6H14N2O2	C00047
glutamine	C5H10N2O3	C00064
O-acetyl-L-serine	C5H9NO4	C00979
glutamate	C5H9NO4	C00025
methionine	C5H11NO2S	C00073
guanine	C5H5N5O	C00242

histidine	C6H9N3O2	C00135
2-Aminooctanoic acid	C8H17NO2	HMDB00991
carnitine	C7H15NO3	C00318
Methionine sulfoxide	C5H11NO3S	HMDB02005
phenylalanine	C9H11NO2	C00079
Pyridoxamine	C8H12N2O2	C00534
pyridoxine	C8H11NO3	C00314
1-Methyl-Histidine	C7H11N3O2	C01152
N-acetyl-L-ornithine	C7H14N2O3	C00437
arginine	C6H14N4O2	C00062
citrulline	C6H13N3O3	C00327
N-carbamoyl-L-aspartate	C5H8N2O5	C00438
glucosamine	C6H13NO5	C00329
tyrosine	C9H11NO3	C00082
Phosphorylcholine	C5H15NO4P	C00588
3-phospho-serine	C3H8NO6P	C01005
N6-Acetyl-L-lysine	C8H16N2O3	C02727
Acetyllysine	C8H16N2O3	C02727
N-acetyl-glutamine	C7H12N2O4	HMDB06029
N-acetyl-glutamate	C7H11NO5	C00624
Ng,NG-dimethyl-L-arginine	C8H18N4O2	C03626
Acetylcarnitine DL	C9H18NO4	C02571
tryptophan	C11H12N2O2	C00078
Kynurenine	C10H12N2O3	C00328
N-acetyl-glucosamine	C8H15NO6	C00140
Flavone	C15H10O2	C15608
cystathionine	C7H14N2O4S	C00542
5-methoxytryptophan	C12H14N2O3	HMDB02339
Cystine	C6H12N2O4S2	C00491
cytidine	C9H13N3O5	C00475
biotin	C10H16N2O3S	C00120
deoxyadenosine	C10H13N5O3	C00559
Glycerophosphocholine	C8H21NO6P	C00670
acadesine	C9H14N4O5	D02742
D-glucosamine-6-phosphate	C6H14NO8P	C00352
D-glucosamine-1-phosphate	C6H14NO8P	C03783
thiamine	C12H16N4OS	C00378
S-ribosyl-L-homocysteine_pos	C9H17NO6S	C03539
deoxyguanosine	C10H13N5O4	C00212
adenosine	C10H13N5O4	C00212
1-Methyladenosine	C11H15N5O4	C02494
guanosine	C10H13N5O5	C00387
L-arginino-succinate	C10H18N4O6	C03406
S-methyl-5-thioadenosine	C11H15N5O3S	C00170
7-methylguanosine	C11H16N5O5	HMDB01107
dCMP	C9H14N3O7P	C00239
glutathione	C10H17N3O6S	C00051
dTMP	C10H15N2O8P	C00364
CMP	C9H14N3O8P	C00055
UMP	C9H13N2O9P	C00105
dAMP	C10H14N5O6P	C00360
Nicotinamide ribotide	C11H15N2O8P	C00455

aminoimidazole carboxamide ribonucleotide	C9H15N4O8P	C04677
thiamine-phosphate	C12H17N4O4PS	C01081
dGMP	C10H14N5O7P	C00362
AMP	C10H14N5O7P	C00020
IMP	C10H13N4O8P	C00130
S-adenosyl-L-methioninamine	C14H23N6O3S	C01137
GMP	C10H14N5O8P	C06193
xanthosine-5-phosphate	C10H13N4O9P	C00655
riboflavin	C17H20N4O6	C00255
S-adenosyl-L-homoCysteine_pos	C14H20N6O5S	C00021
S-adenosyl-L-methionine	C15H22N6O5S	C00019
folate	C19H19N7O6	C00504
7,8-dihydrofolate	C19H21N7O6	C00415
5-methyl-THF	C20H25N7O6	C00440
Diiodothyronine	C15H13I2NO4	HMDB00582
glutathione disulfide_pos	C20H32N6O12S2	C00127
NAD+_pos	C21H27N7O14P2	C00003
NADH	C21H29N7O14P2	C00004
dephospho-CoA_pos	C21H35N7O13P2S	C00882
NADP+_pos	C21H28N7O17P3	C00006
NADPH	C21H30N7O17P3	C00005
coenzyme A_pos	C21H36N7O16P3S	C00010
FAD	C27H33N9O15P2	C00016
acetyl-CoA_pos	C23H38N7O17P3S	C00024
propionyl-CoA_pos	C24H40N7O17P3S	C00100
acetoacetyl-CoA_pos	C25H40N7O18P3S	C00332
malonyl-CoA_pos	C24H38N7O19P3S	C00083
succinyl-CoA_pos	C25H40N7O19P3S	C00091
putrescine	C4H12N2	C00134
spermidine	C7H19N3	C00315
spermine	C10H26N4	C00750
sarcosine	C3H7NO2	C00213
