

Metabolite	Category
2-ketoisocaproic acid	amino acid metabolism
2-picolinic acid	amino acid metabolism
3,4-dihydroxyphenylacetic acid	amino acid metabolism
3-phenyllactic acid	amino acid metabolism
4-aminobutyric acid	amino acid metabolism
4-hydroxybenzoate	amino acid metabolism
4-hydroxyphenylacetic acid	amino acid metabolism
5-aminovaleric acid	amino acid metabolism
alanine	amino acid metabolism
alanine-alanine	amino acid metabolism
asparagine	amino acid metabolism
aspartic acid	amino acid metabolism
beta-alanine	amino acid metabolism
cysteine	amino acid metabolism
cystine	amino acid metabolism
glutamine	amino acid metabolism
glutaric acid	amino acid metabolism
glycine	amino acid metabolism
histidine	amino acid metabolism
homocystine	amino acid metabolism
homoserine	amino acid metabolism
indole-3-lactate	amino acid metabolism
isoleucine	amino acid metabolism
leucine	amino acid metabolism
lysine	amino acid metabolism
methionine	amino acid metabolism
methionine sulfoxide	amino acid metabolism
N-acetylaspatic acid	amino acid metabolism
n-acetylglutamate	amino acid metabolism
N-acetylornithine	amino acid metabolism
N-acetylputrescine	amino acid metabolism
N-methylalanine	amino acid metabolism
O-acetylserine	amino acid metabolism
ornithine	amino acid metabolism
phenol	amino acid metabolism
phenylacetic acid	amino acid metabolism
phenylalanine	amino acid metabolism
phenylethylamine	amino acid metabolism
pipecolic acid	amino acid metabolism
proline	amino acid metabolism

putrescine	amino acid metabolism
pyrrole-2-carboxylic acid	amino acid metabolism
serine	amino acid metabolism
shikimic acid	amino acid metabolism
threonine	amino acid metabolism
trans-4-hydroxyproline	amino acid metabolism
tryptophan	amino acid metabolism
tyramine	amino acid metabolism
tyrosine	amino acid metabolism
urea	amino acid metabolism
urocanic acid	amino acid metabolism
valine	amino acid metabolism
N-acetyl-D-galactosamine	amino sugar
n-acetyl-d-hexosamine	amino sugar
chenodeoxycholic acid	bile acid
cholic acid	bile acid
taurine	bile acid
aconitic acid	central metabolism
alpha-ketoglutarate	central metabolism
citramalic acid	central metabolism
citric acid	central metabolism
dihydroxyacetone	central metabolism
fumaric acid	central metabolism
glucose-6-phosphate	central metabolism
glyceric acid	central metabolism
isocitric acid	central metabolism
malic acid	central metabolism
oxalic acid	central metabolism
pyrophosphate	central metabolism
pyruvic acid	central metabolism
succinic acid	central metabolism
sulfuric acid	central metabolism
2-hydroxybutanoic acid	fatty acid
arachidic acid	fatty acid
arachidonic acid	fatty acid
behenic acid	fatty acid
capric acid	fatty acid
cerotinic aci	fatty acid
elaidic acid	fatty acid
heptadecanoic acid	fatty acid
isoheptadecanoic acid NIST	fatty acid

lauric acid	fatty acid
lignoceric acid	fatty acid
linoleic acid	fatty acid
myristic acid	fatty acid
nonadecanoic acid	fatty acid
oleic acid	fatty acid
palmitic acid	fatty acid
pentadecanoic acid	fatty acid
stearic acid	fatty acid
butane-2,3-diol NIST	fermentation product
lactic acid	fermentation product
1-monoheptadecanoyl glyceride NIST	lipid metabolism
1-monoolein	lipid metabolism
1-monopalmitin	lipid metabolism
1-monostearin	lipid metabolism
2-monoolein	lipid metabolism
2-monopalmitin	lipid metabolism
dodecanol	lipid metabolism
ethanolamine	lipid metabolism
glycerol-alpha-phosphate	lipid metabolism
monomyristin	lipid metabolism
phosphoethanolamine	lipid metabolism
phytol	lipid metabolism
propane-1,3-diol NIST	lipid metabolism
3-aminoisobutyric acid	nucleotide metabolism
3-hydroxypropionic acid	nucleotide metabolism
5,6-dihydrouracil	nucleotide metabolism
7-methylguanine NIST	nucleotide metabolism
adenine	nucleotide metabolism
adenosine	nucleotide metabolism
adenosine-5-monophosphate	nucleotide metabolism
cytosin	nucleotide metabolism
guanosine	nucleotide metabolism
inosine	nucleotide metabolism
orotic acid	nucleotide metabolism
pseudo uridine	nucleotide metabolism
ribose	nucleotide metabolism
thymidine	nucleotide metabolism
thymine	nucleotide metabolism
uracil	nucleotide metabolism
uric acid	nucleotide metabolism
uridine	nucleotide metabolism

xanthine	nucleotide metabolism
xanthosine	nucleotide metabolism
2,3-dihydroxybutanoic acid NIST	organic acid
2-deoxytetrionic acid	organic acid
2-deoxytetrionic acid NIST	organic acid
2-hydroxyglutaric acid	organic acid
2-hydroxyhexanoic acid	organic acid
2-hydroxyvaleric acid	organic acid
3-hydroxy-3-methylglutaric acid	organic acid
3-hydroxybutyric acid	organic acid
adipic acid	organic acid
azelaic acid	organic acid
benzoic acid	organic acid
digalacturonic acid	organic acid
erythronic acid lactone	organic acid
glycolic acid	organic acid
hexaric acid	organic acid
maleic acid	organic acid
syringic acid	organic acid
tartaric acid	organic acid
cholesterol	sterol
dihydrocholesterol	sterol
squalene	sterol
stigmasterol	sterol
beta-gentiobiose	sugar
cellobiose	sugar
fructose	sugar
glucose	sugar
glycerol-3-galactoside	sugar
levoglucosan	sugar
lyxose	sugar
maltose	sugar
maltotriose	sugar
mannose	sugar
N-acetyl-D-mannosamine	sugar
raffinose	sugar
tagatose	sugar
trehalose	sugar
xylose	sugar
xylulose NIST	sugar
galacturonic acid	sugar acid
gluconic acid	sugar acid

gluconic acid lactone	sugar acid
lactobionic acid	sugar acid
ribonic acid	sugar acid
saccharic acid	sugar acid
threonic acid	sugar acid
UDP-glucuronic acid	sugar acid
xylonic acid	sugar acid
erythritol	sugar alcohol
erythrose	sugar alcohol
fucose	sugar alcohol
galactinol	sugar alcohol
hexitol	sugar alcohol
isothreitol	sugar alcohol
lactitol	sugar alcohol
lyxitol	sugar alcohol
mannitol	sugar alcohol
palatinitol	sugar alcohol
xylitol	sugar alcohol
4-pyridoxic acid	vitamin metabolism
delta-tocopherol NIST	vitamin metabolism
hexuronic acid1	vitamin metabolism
nicotinamide	vitamin metabolism
nicotinic acid	vitamin metabolism
tocopherol alpha-	vitamin metabolism
tocopherol beta NIST	vitamin metabolism
tocopherol gamma-	vitamin metabolism
1,2-anhydro-myo-inositol NIST	xother
2-deoxypentitol NIST	xother
2-hydroxypyrazinyl-2-propenoic acid ethyl ester NIST	xother
4-hydroxymandelic acid	xother
5-hydroxymethyl-2-furoic acid NIST	xother
6-hydroxynicotinic acid	xother
acetophenone NIST	xother
allantoic acid	xother
alloxanoic acid NIST	xother
aminomalonate	xother
beta-mannosylglycerate	xother
butyrolactam NIST	xother
caffeine	xother
conduritol-beta-epoxide	xother
creatinine	xother
docosahexaenoic acid	xother

epsilon-caprolactam	xother
hexadecylglycerol NIST	xother
hydroxycarbamate NIST	xother
hydroxylamine	xother
indole-3-acetate	xother
inositol-4-monophosphate	xother
isohexonic acid	xother
isothreonic acid	xother
maleimide	xother
malonic acid	xother
methyl O-D-galactopyranoside	xother
methyltetrahydrophenanthrene1 NIST	xother
parabanic acid NIST	xother
sebacic acid, di(2-octyl) ester NIST	xother
tyrosol	xother
xylonolactone NIST	xother
zymosterol	xother