

Full panel run at UCSD Biochemical Genetics Laboratory (2 runs using both ionization modes)

Negative ionization run

2-decenedioic
2-ethyl-3-hydroxypropionic
2-hydroxy-3-methylvaleric
2-hydroxyadipic
2-hydroxybutyric
2-hydroxyglutaric
2-hydroxyisocaproic
2-hydroxyisovaleric
2-hydroxyphenylacetic
2-hydroxysebacic
2-methylacetoacetic
2-methylbutyrylglycine
2-methylcitric
2-octenedioic
2-oxoadipic
2-oxobutyric
2-oxoglutaric
2-oxoisocaproic
2-oxoisovaleric
3-(3-MeO-4-OH)phenyllactic
3-(3-OH-phenyl)-3-OH-propionic
3-hydroxy-2-methylbutyric
3-hydroxy-3-methylglutaric
3-hydroxyadipic
3-hydroxyadipic_lactone
3-hydroxybutyric
3-hydroxydecanedioic
3-hydroxyglutaric
3-hydroxyisobutyric
3-hydroxyisovaleric
3-hydroxypropionic
3-hydroxysebacic
3-hydroxyvaleric
3-methyladipic
3-methylcrotonylglycine
3-methylglutaconic
3-methylglutaric
4-hydroxybutyric

Positive ionization run

(2/3)-amino(iso)butyric acid
(3/5)-methylcytidine
1,7-dimethylxanthine
1-alpha,25-dihydroxyvitamin D3
1-methylhistidine
2-aminobutyric
2-deoxyadenosine
2-deoxycytidine
2-deoxyguanosine
2-deoxyinosine
2-deoxyuridine
2-methylbutyrylcarnitine
25-hydroxyvitamin D2
25-hydroxyvitamin D3
3-methylhistidine
4-aminobutyric
4-hydroxyproline
4-pyridoxic_lactone
5-aminolevulinic
5-Hydroxymethyluracil
5-hydroxypipercolic
5-methylcytidine
7,8-dihydrobiopterin
7-methylguanine
7-methylguanosine
acetylcarnitine
acetylcholine
adenine
adenosine
adenylosuccinic
AICAR
AICARiboside
alanine
allo+delta-Hydroxylysine
allopurinol
allopurinol-riboside
alpha-amino-gamma-guanidinobutyric
alpha-aminoadipic acid

4-hydroxycyclohexylacetic	alpha-aminobutyric
4-hydroxyhippuric	alpha-CEHC (carboxyethylhydroxychroman)
4-hydroxyisovaleric	alpha-tocopherol
4-hydroxyphenylacetic	alpha-tocopherol_acetate
4-hydroxyphenyllactic	aminoimidazolecarboximide (AICA)
4-hydroxyphenylpyruvic	anserine
4-pyridoxic	arabinose/ribose/xylose (aldopentoses)
5-hydroxyhexanoic	arabitol/ribitol/xylitol (C5 sugar alcohols)
5-Hydroxyindoleacetic	arginine
5-oxoproline	argininosuccinic
7-hydroxyoctanoic	asparagine
acetoacetic	aspartic acid
aconitic-Z	asym-dimethylarginine
adipic	beta-alanine
allantoin	betaine
ascorbic	biopterin
azelaic	biotin
benzoic	butyrylcarnitine
butyrylglycine	butyrylcholine
cinnamoylglycine-trans	cadaverine
citric	caffeine
dodecanedioic	canavanine
ethylmalonic	carnitine
fumaric	carnosine
furan-2,5-dicarboxylic	choline
glutaconic	citrulline
glutaric	creatine
glyceric	creatinine
glycochenodeoxycholic	cystathionine
glycocholic	cysteine
glycodeoxycholic	cysteinylglycine
glycolic	cystine
glyoxylic	cytidine
hexanoylglycine	cytosine
hexose	decanoylcarnitine
hippuric	delta-tocopherol
homogentisic	dihydroorotic
homovanillic	dihydrothymine
indole-3-acetic	dihydrouracil
indole-3-aldehyde	dimethylglycine
indole-3-carboxylic	dopamine
indole-3-propionic	epinephrine
indole-3-pyruvic	folic

indolelactic	fucose (deoxyhexose)
isobutyrylglycine	galactitol/mannitol/sorbitol (C6 sugar alcohols)
isocitric	gamma-aminobutyric acid
isovaleryl-glycine	gamma-butyrobetaine
kynurenic	gamma-CEHC
lactic	gamma-tocopherol
maleic	glucosamine
malic	glucosamine and galactosamine
	glucose/ galactose/ mannose/ fructose (aldohexoses, and keto-hexose (fructose))
malonic	glucuronic acid (and lactone)
methylmalonic	glutamic acid
methylsuccinic	glutamine
mevalonic	glycine
mevalonolactone	glycylglycine
N-acetyl-aspartic	glycylproline
N-acetyl-tyrosine	guanidinoacetic
orotic acid	guanine
oxalic	guanosine
pantothenic	hexanoylcarnitine
phenylacetic	histamine
phenyllactic	histidine
phenylpyruvic	homoarginine
pimelic	homocitrulline
propionylglycine	homocysteine
pyruvic	homocystine
quinolinic	hypoxanthine
sebacic	indole-3-butyric
suberic	inosine
suberylglycine	isobutyrylcarnitine
succinic	isoleucine
succinic semialdehyde	isovalerylcarnitine
succinylacetone	isoxanthopterin
tetradecanedioic	kynurenine
tiglylglycine	L-DOPA
tridecanedioic	lauroylcarnitine
undecanedioic	lauroylcholine
uracil	leucine
uric	lysine
urocanic	melatonin
valeryl-glycine	methionine
vanillylmandelic	MHPG (4-hydroxy-3-methoxyphenylglycol)
	monapterin

myo-inositol (cyclic C6 sugar alcohol)
myristoylcarnitine
myristoylcholine
N-acetyl-neuraminic (incl. sialic acid, amino oligosaccharide)
N-acetylglucosamine/ N-acetylgalactosamine
neopterin
niacin
norepinephrine
O-phosphoethanolamine
octanoylcarnitine
ornithine
oxipurinol
palmitoylcarnitine
paraxanthine
penicillamine
phenylalanine
pipercolic
proline
propionylcarnitine
propionylcholine
pseudouridine
pterin
putrescine
riboflavin
ribothymidine
ribulose (ketopentose)
S-adenosylhomocysteine
S-adenosylmethionine
SAICAR
sarcosine
sepiapterin
serine
serotonin
spermidine
spermine
stearoylcarnitine
succinyladenosine
sym-dimethylarginine
taurine
tetrahydrofolic
theobromine
theophylline
thiamine

threonine
thymidine
thymine
trimethyl-lysine
trimethylamine
trimethylamine-n-oxide
tryptamine
tryptophan
tyramine
tyrosine
ureidopropionic
uridine
valerylcarnitine
valine
vitamin D3 sulfate
xanthine
xanthosine