

Supplemental materials

Supplemental Table 1: Metabolites measured within the sample set

1-methylhistamine	dodecenoylcarnitine (C12:1 carnitine)	glucuronate	myristoylcarnitine (14:0 carnitine)	thymine
1-methylnicotinamide	tetradecenoylcarnitine (C14:1 carnitine)	glutamate	N-carbamoyl-beta-alanine	thyroxine
2,3-phosphoglycerate	tetradecenoylcarnitine (C14:1 carnitine)	glutamine	niacinamide	triiodothyronine
2-aminoadipate	tetradecadienoylcarnitine (C14:2 carnitine)	glycine	NMMA	trimethylamine-N-oxide
2-hydroxyglutarate	palmitoylcarnitine (C16 carnitine)	glycocholate	nonanoylcarnitine (9:0 carnitine)	tryptophan
3-hydroxyanthranilic acid	3-Hydroxypalmitoylcarnitine (C16-OH carnitine)	glycodeoxycholate;	octanoylcarnitine (8:0 carnitine)	tyrosine
3-hydroxykynurenate	3-hydroxyoleoylcarnitine (C18:1-OH carnitine)	glycochenodeoxycholate	oleoylcarnitine (18:1 carnitine)	uracil
3-methyladipate; pimelate	arachidoyl carnitine, eicosanoyl carnitine (C20 carnitine)	guanosine	ornithine	urate
4-hydroxybenzaldehyde	malonylcarnitine (C3-DC carnitine)	heptanoylcarnitine (7:0 carnitine)	orotate	uridine
4-hydroxymandelate	C3-DC-CH3 carnitine	hexacosanoylcarnitine (26:0 carnitine)	oxalate	valerylcarnitine (5:0 carnitine)
4-pyridoxate	3-hydroxy-butyl carnitine (C4-OH carnitine)	hexanoylcarnitine (6:0 carnitine)	pantothenate	valine
5-adenosylhomocysteine	tyglyl carnitine (C5:1 carnitine)	hexose monophosphate	p-cresol sulfate	vanillylmandelic acid (VMA)
5-aminolevulinic acid	glutaryl carnitine (C5-DC carnitine)	hippurate	pentose monophosphate	xanthine
acetylcarnitine (2:0 carnitine)	carnitine	histamine	phenylalanine	xanthosine
aconitate	choline	histidine	phosphocholine	xanthurena
adenine	citrate	homocysteine	phosphocreatine	
adenosine	citruiline	homogentisate	phosphoethanolamine	
adipate	cotinine	hydroxyphenylacetate	pipecolic acid	
alanine	creatine	hydroxyproline	proline	
allantoin	creatinine	hypoxanthine	propionate	
alpha-glycerophosphate	cystathionine	indole-3-propionate	propionylcarnitine (3:0 carnitine)	
alpha-glycerophosphocholine	cytidine	indolelactate	putrescine	
alpha-hydroxybutyrate	deoxycytidine monophosphate (dCMP)	indoxy sulfate	pyroglutamic acid	
aminoisobutyric acid	decanoylcarnitine (10:0 carnitine)	inosine	quinolinate	
anserine	dimethylglycine	inositol	s-adenosylmethionine	
anthranilic acid	deoxyuridine monophosphate (dUMP)	isocitrate	salicylurate	
arachidonyl carnitine (20:4 carnitine)	fructose/glucose/galactose	isoleucine	sarcosine	
arginine	fumarate; maleate 1	kynurenine	serine	
asparagine	fumarate; maleate 2	lactate	serotonin	
aspartate	gamma-aminoisobutyric acid	lactose	sorbitol	
asymmetric dimethyl-arginine (ADMA)	gentisate	lauroylcarnitine (12:0 carnitine)	spermidine	
beta-alanine	glucose	leucine	stearoylcarnitine (18:0 carnitine)	
beta-hydroxybutyrate		linoleylcarnitine (18:2 carnitine)	suberate	
betaine		lithocholate	succinate	
bilirubin		lysine	sucrose	
butyrobetaine		malate	symmetric dimethyl-arginine (SDMA)	
butyrylcarnitine (4:0 carnitine)		methionine	taurine	
decadienoyl carnitine (C10:2 carnitine)		methionine sulfoxide	taurodeoxycholate;	
		methyImalonate	taurochenodeoxycholate	
		methyIthioadenosine	thiamine	
			threonine	