Electronic Supplementary Material

New markers for sepsis caused by *Pseudomonas aeruginosa* during burn infection

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Online Resource 3: Table 3 Classification and functional pathways for, or sources of, the 148 identified metabolites

Metabolite	Synonyms	Class	Pathway or source
Purine Derivatives			
1-methylinosine		modified nucleotide	purine metabolism
allantoic acid	allantoate	*N*- carbamoyl-alpha amino acids	purine metabolism (uric acid)
uric acid	urate	heterocyclic purine deravitives, xanthines	purine metabolism
Pyrimidines and Derivatives			
3-aminoisobutyric acid	3-amino-2-methylpropanoic acid, beta-aminoisobutyric acid	beta amino acids	pyrimidine degradation
3-ureidopropionate[a]	3-ureidopropionate, *N*-carbamoyl-β-alaninate	ureas	pyrimidine (uracil) metabolism
β-alanine	3-aminopropanoic acid, 3-aminopropionic acid	beta amino acids and derivatives	pyrimidine metabolism; amino acid metabolism (Asp, His),
orotic acid	6-carboxyuracil, orotate	pyrimidines and pyrimidine derivatives	pyrimidine metabolism
pseudouridine	pseudouridine, β-pseudouridine, psi-uridine	nucleoside/nucleotide analogs	pyrimidine metabolism
thymidine		pyrimidine nucleosides	pyrimidine metabolism
thymine	5-methyluracil	hydroxypyrimidines	pyrimidine metabolism
uracil		pyrimidones	pyrimidine metabolism
uridine		pyrimidine nucleosides	pyrimidine metabolism
Fatty Acids and Lipid Metabolites			
1-monoolein	2,3-dihydroxypropyl oleate, glycerolmonooleate, monooleoylglycerol	lipid; monoacylglycerides	lipid metabolism

3,4-dihydroxybutyric acid	3,4-dihydroxybutanoic acid; 2-deoxytetronic acid	fatty acids (omega hydroxy)	fatty acid (butyric acid) metabolism
3-hydroxybutyric acid	3-hydroxybutanoic acid, β-hydroxybutyric acid	beta hydroxy acids	fatty acid metabolism
4-hydroxybutyric acid	4-hydroxybutanoic acid, γ-hydroxybutyric acid	short-chain fatty acid	fatty acid metabolism (GABA precursor)
arachidic acid	eicosanoic acid	long-chain fatty acids	lipid metabolism
arachidonic acid	arachidonate	long-chain fatty acids	fatty acid metabolism; arachidonic acid metabolism
β-glycerophosphate	glycerol-2-phosphate, 2-glycerophosphate	glycerophosphates	glycerolipid metabolism
butane-2,3-diol [NIST]	2,3-butanediol	1,2-diol, aliphatic hydrocarbon	gut microbial metabolite
capric acid	decanoic acid	medium-chain fatty acid	fatty acid metabolism
cholesterol		lipid, sterol	lipid metabolism; steroid biosynthesis; bile acid biosynthesis
citraconic acid	2-methylmaleic acid, methylmaleic acid	methyl-branched-chain fatty acids	microbial metabolite
dodecanol	1-dodecanol	fatty alcohols	lipid metabolism
ethanolamine	2-aminomethanol	aminoalcohol	phospholipid biosynthesis
glyceric acid	DL-glyceric acid	sugar acids and derivatives	glycerolipid metabolism, amino acid (Gly, Ser) metabolism
glycerol	glycerine	sugar alcohols	glycerolipid metabolism, CHO (galactose) metabolism
glycerol-1-phosphate	glycerol-3-phosphate, glycerol-α-phosphate, glycerophosphoric acid	glycerophosphates	glycerol phosphate shuttle, glycerolipid metabolism, phospholipid biosynthesis
glycerol-3-galactoside	glycerol-3-galactose, 3-β-D-galactosyl-*sn*-glycerol, galactosylglycerol	glycosoglycerols	glycerolipid metabolism; CHO (galactose) metabolism
lauric acid	dodecanoic acid	medium chain fatty acids	fatty acid metabolism
linoleic acid	linolic acid, linoleate	fatty acids	fatty acid metabolism
myristic acid	tetradecanoic acid	long-chain fatty acids	fatty acid metabolism
nonadecanoic acid		long-chain fatty acids	fatty acid metabolism
octadecanol	1-octadecanol, stearyl alcohol	long-chain fatty alcohols	glycerophospholipid (plasmalogens) synthesis
oleic acid	*cis*-9-octadecenoic acid, *cis*-oleic acid	long-chain fatty acids	fatty acid metabolism

palmitic acid	hexadecanoic acid, palmitate	long-chain fatty acids	fatty acid metabolism, glycerolipid metabolism
palmitoleic acid	*cis*-9-hexadecenoic acid	long-chain fatty acids	fatty acid metabolism
pelargonic acid	nonanoic acid, pelargic acid, nonanoate	medium-chain fatty acids	fatty acid metabolism
stearic acid	octadecanoic acid	long-chain fatty acids	glycerophospholipid (plasmalogens) synthesis
Amino Acids and Protein Derivatives			
2-hydroxybutyric acid	2-hydroxybutanoic acid, α-hydroxybutyrate	alpha hydroxy acids	amino acid catabolism (Thr, Met) and biosynthesis (Cys)
5-methoxytryptamine	*o*-methylserotonin	tryptamines and derivatives	melatonin degradation; Trp metabolism
5-oxoproline	oxoproline, pyroglutamic acid	alpha amino acids	amino acid metabolism, glutathione metabolism
alanine	L-alanine	amino acids	amino acid metabolism; urea cycle; multiple pathways
α-aminoadipic acid	2-aminohexanedioic acid; 2-aminoadipic acid	alpha-amino acid	amino acid (Lys) metabolism
aminomalonate	2-aminomalonic acid, aminomalonic acid	alpha-amino acids	amino acid (Gly, Ala) metabolism
asparagine	L-asparagine	amino acids	amino acid metabolism
aspartate	aspartic acid	amino acids	amino acid metabolism; urea cycle
benzoate	benzoic acid	benzoic acids	microbial metabolite (Phe)
β-glutamic acid	3-aminopentanedioic acid, 3-aminoglutaric acid, isoglutamic acid	beta-amino acids	microbial metabolite
citrulline	L-citrulline	L-alpha-amino acids	amino acid metabolism (Arg, Pro, Asp); urea cycle
creatinine		alpha amino acids	protein degradation
cysteine	L-cysteine	amino acids	amino acid metabolism (Cys, Glu, Gly, Ser, Met), glutathione metabolism; taurine metabolism
glutamate	glutamic acid	amino acids	amino acid metabolism
glutamine	L-glutamine	amino acids	amino acid metabolism
glutarate	glutaric acid, pentanedioic acid	dicarboxylic acids	amino acid metabolism (Lys, Trp)
glycine	2-aminoacetic acid	amino acids	amino acid (Ala, Gly, Ser, Arg, Pro) metabolism, multiple pathways

hippurate	hippuric acid, 2-benzamidoacetic acid	benzoic acids and derivatives	amino acid (Gly) metabolism
histidine	L-histidine	amino acids	amino (His, β-Ala) acid
homoserine	L-homoserine	amino acids	amino acid (Met) metabolism
hydroxylamine	hydroxyamine	inorganic compound	waste product, related to ammonia
indole-3-acetate	indoleacetic acid, 3-indoleaceticacid	indoxyl carboxylic acids and derivatives	gut microbial metabolite (Trp)
indole-3-lactate	indolelactic acid, 3-indolelactate	indoxyl carboxylic acids and derivatives	amino acid (Trp) metabolism
indole-3-propionate	indolepropionate, indole-3-propionic acid	indoxyl carboxylic acids and derivatives	gut microbial metabolite (Trp)
isoleucine	L-isoleucine	amino acids	amino acid metabolism
leucine	L-leucine	amino acids	amino acid (Val, Leu, Ile) metabolism
lysine	L-lysine	amino acids	amino acid (Lys) metabolism, carnitine synthesis
methionine	L-methionine	amino acids	amino acid (Met, Gly, Ser) metabolism
methionine sulfoxide	L-methionine sulfoxide	L-alpha-amino acids	amino acid (Met) metabolism
ornithine	L-ornithine	amino acids	amino acid (Arg, Pro, Gly, Ser) metabolism, urea cycle
phenylalanine	L-phenylalanine	amino acids	amino acid (Phe, Tyr) metabolism
p-tolyl glucuronide	*p*-cresol glucuronide, *p*-tolyl-D-glucuronide, *p*-tolyl-β-D-glucuronide, *p*-cresyl glucuronide	phenolic glycosides	microbial metabolite (Tyr)
serine	L-serine	amino acids	amino acid (Gly, Ser, Met) metabolism, sphingolipid metabolism, ammonia recycling
taurine	2-aminoethanesulfonic acid, L-taurine	organosulfonic acid, sulfur amino acid	amino acid (Tau, hypotaurine) metabolism; bile acid biosynthesis
threonine	L-threonine	amino acids	amino acid (Gly, Ser, Thr) metabolism
***trans*-4-hydroxyproline**	L-hydroxyproline, 4-hydroxyproline	proline and derivatives	protein (collagen) metabolism
tryptophan	L-tryptophan	L-alpha-amino acids	amino acid (Trp) metabolism

tyrosine	L-tyrosine	L-alpha-amino acids	amino acid (Tyr, Phe) metabolism
urea	isourea, carbamide	ureas	urea cycle, amino acid (Arg, Pro) metabolism
valine	L-valine	amino acids	amino acid (Val, Leu, Ile) metabolism
Vitamins and Derivatives, Phosphate, and Metabolites of Unknown Function			
α-tocopherol	vitamin E	tocopherols	vitamin
oxalate	oxalic acid, ethanedioic acid	dicarboxylic acids	ascorbic acid metabolism, glyoxylic acid metabolism
pantothenic acid	D-pantothenic acid, vitamin B5	secondary alcohols	vitamins/cofactors
threonate	threonic acid, isothreonic acid	sugar acids and derivatives	ascorbate and aldarate metabolism
phosphate	orthophosphate, phosphate ion, Pi	non-metal phosphates	multiple synthetic and degradative pathways
hydroxycarbamic acid	hydroxycarbamate		unknown
methyl dihydrogen phosphate	methanolphosphate, methylphosphate	monoalkyl phosphates	unknown
Sugars, Sugar Acids, Sugar Alcohols, and Carbohydrate Metabolites			
3,6-anhydro-D-galactose[b]	3,6-anhydrogalactose	hexose	CHO metabolism; mouse metabolite
3-phosphoglycerate	glycerate-3-phosphate	sugar acids and derivatives	glycolysis
altrose	L-altrose	aldohexose	microbial metabolite
arabitol	D-arabinitol	polyols (sugar alcohols)	pentose phosphate pathway
fructose	D-fructose, D-fructopyranose	pentose	carbohydrate (CHO) metabolism
fructose-6-phosphate		hexose phosphate	glycolysis, gluconeogenesis, CHO metabolism
fucose	L-fucose, 6-deoxy-L-galactose	hexose deoxy sugar	CHO (fructose, mannose) metabolism
gluconate	gluconic acid	sugar acids and derivatives	CHO (glucose) metabolism
glucose	D-glucose	hexose	glucolysis, gluconeogenesis
glucose-6-phosphate	D-glucose-6-phosphate	hexose phosphate	glycolysis, gluconeogenesis, multiple pathways
hexitols	Multiple hexitols: D-mannitol, D-sorbitol, D-galactitol	sugar alcohols	Fructose/mannose degradation, galactose metabolism
hexose-6-phosphate	D-hexose 6-phosphate	hexose phosphates	pentose phosphate pathway

hexuronic acids	one of 25 different types: in humans: e.g., glucuronic acid	glucuronic acid derivatives	CHO (inositol, starch, sucrose) metabolism
isothreonic acid	threonic acid, D-threonic acid	sugar acids and derivatives	microbial metabolite (ascorbic acid)
lactate	lactic acid	alpha hydroxy acids	gluconeogenesis, pyruvate fermentation
lactose		*o*- glycosyl compounds	CHO (lactose, galactose) metabolism
lyxitol	D-arabinitol	sugar alcohols	pentose/glucuronate interconversion pathway
lyxose	D-lyxose, pectin, galacturonate	glucuronic acid derivatives	pentose phosphate pathway
mannitol		sugar alcohols	CHO (fructose) metabolism
mannose	D-mannose	hexose	CHO (fructose, mannose, galactose) metabolism
myo -Inositol	L-inositol	cyclohexanol	CHO (galactose) metabolism, phosphatidylinositol phosphate metabolism
N -acetyl-d-hexosamines	group of compounds (e.g. *N* -acetyl-D-glucosamine, *N* -acetyl-D-mannosamine)	acylaminosugars	amino sugar metabolism
N -acetylmannosamine	*N* -acetyl-D-mannosamine	acylaminosugars	amino sugar metabolism
phosphoenolpyruvate	phosphoenolpyruvic acid	phosphate esters	glycolysis, gluconeogenesis, multiple pathways
pyruvate	2-oxopropanoic acid, 2-oxopropionic acid, pyruvic acid	alpha-keto acids and derivatives	gluconeogenesis, glycolysis, amino sugar metabolism, TCA cycle, amino acid (Ala, Gly, Ser, Cys, Glu) metabolism, pyruvate metabolism, urea cycle
ribitol	*meso*- adonitol, adonitol	sugar alcohols	ribose metabolism
ribonic acid	D-ribonate	sugar acids and derivatives	ribose metabolism
ribose	D-Ribose, D-ribofuranose	pentoses	pentose phosphate pathway
sorbitol	D-Sorbitol, D-glucitol	sugar alcohols	CHO metabolism
sucrose		*o*- glycosyl compounds	CHO (starch, sucrose, galactose) metabolism
tagatose	D-Tagatose	monosaccharides	CHO metabolism
threitol	D-Threitol	sugar alcohols	CHO (xylose) metabolism
trehalose	D-Trehalose, mycose	*o*- glycosyl compounds	CHO (trehalose) degradation
xylose	D-xylose	pentoses	CHO (anionic polysaccharides) metabolism

Tricarboxylic Acid Cycle Intermediates			
2-hydroxyglutarate	2-hydroxyglutaric acid	short-chain hydroxy acids	TCA cycle offshoot
α-ketoglutarate	2-ketoglutaric acid, 2-oxoglutaric acid; oxoglutaric acid	gamma-keto acids and derivatives	TCA cycle; multiple pathways
cis-aconitate	*cis*-aconitic	tricarboxylic acids and derivatives	TCA cycle
citramalate	citramalic acid	hydroxy fatty acid	TCA cycle (analog of malic acid); amino acid metabolism (Ile)
citrate	citric acid	tricarboxylic acids and derivatives	TCA cycle
fumarate	fumaric acid, 2-butenedioic acid	dicarboxylic acids	TCA cycle; multiple pathways
glycolate	glycolic acid, 2-hydroxyacetic acid,	alpha-hydroxy acids	metabolic acidosis (with oxalic acid, lactic acid); regulation by TCA enzymes
isocitrate	isocitric acid	tricarboxylic acids and derivatives	TCA cycle
itaconic acid	itaconate, 2-methylenesuccinic acid	branched fatty acids	TCA cycle (derivative of succinic acid)
malate	malic acid	beta hydroxy acids	TCA cycle, multiple pathways
succinate	succinic acid, butanedioic acid	dicarboxylic acids	TCA cycle, amino acid (Glu, Val, Leu, Ile) glutamate metabolism, carnitine synthesis, ketone body metabolism, fatty acid oxidation
Xenobiotics (food, drugs, environment)			
1,3,5-trimethylcyanuric acid	cyanuric acid, isocyanuric acid, trihydroxycyanidine	1,3,5-triazines	xenobiotic
2-deoxy-D-ribitol	2-deoxypentitol [NIST]	secondary alcohols	xenobiotic
4-methylbenzenesulfonamide[b]	*p*-toluenesulfonamide	sulfonamide	xenobiotic
β-sitosterol		phytosterol	xenobiotic
cis-gondoic acid	11Z-eicosenoic acid, gondoic acid	long-chain fatty acids	xenobiotic
conduritol-β-expoxide[b]	1,2-anhydro-*myo*-inositol	conduritol derivative	xenobiotic
ε-caprolactam	caprolactam, azepan-2-one	caprolactams	xenobiotic
heptadecanoic acid		fatty acids (exogenous)	xenobiotic
isobutene glycol [NIST]	2-methylpropane-1,2-diol	primary alcohol, glycol,	xenobiotic metabolite
lactamide	2-hydroxypropanamide	monocarboxylic acid amide	lactic acid derivative
lactulose		*o*-glycosyl compounds	xenobiotic
metharbital	methylbarbital	barbituric acid derivatives	xenobiotic (drug)
pentobarbital [NIST]	nembutal	pyrimidones	xenobiotic (drug)

pinitol	D-pinitol	cyclohexanols	xenobiotic (food)
quinic acid	quinate	quinic acids and derivatives	xenobiotic (food)
raffinose	melitose	oligosaccharides	xenobiotic (food)
xylitol		sugar alcohols	xenobiotic (food)

Abbreviations: CHO, carbohydrate; standard 3-letter codes for amino acids; TCA, tricarboxylic acid cycle (aka, citric acid cycle)

[a]Metabolites in bold in colored boxes were included in the set of potential diagnostic biomarkers

[b]Metabolites that have not been found in humans; these were excluded from the set of potential diagnostic biomarkers