Electronic Supplementary Material

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

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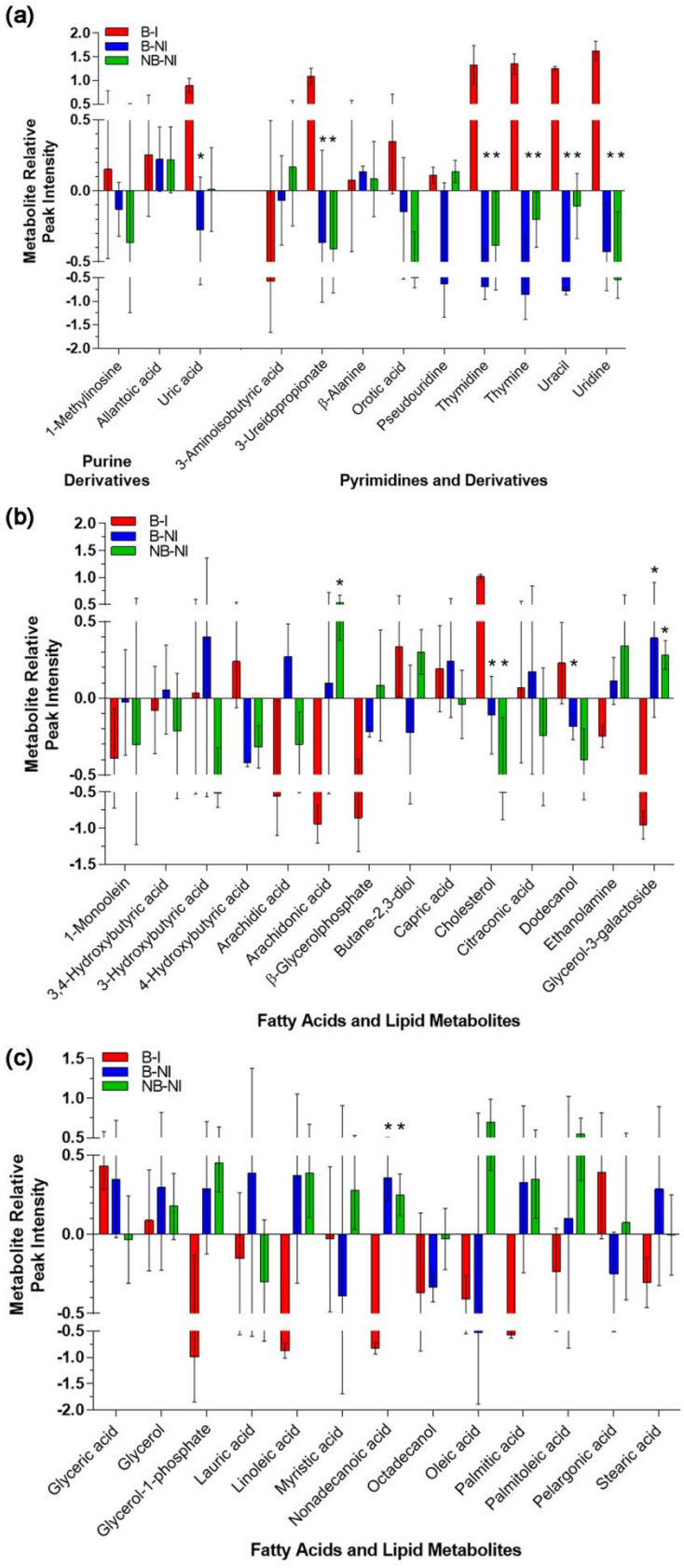
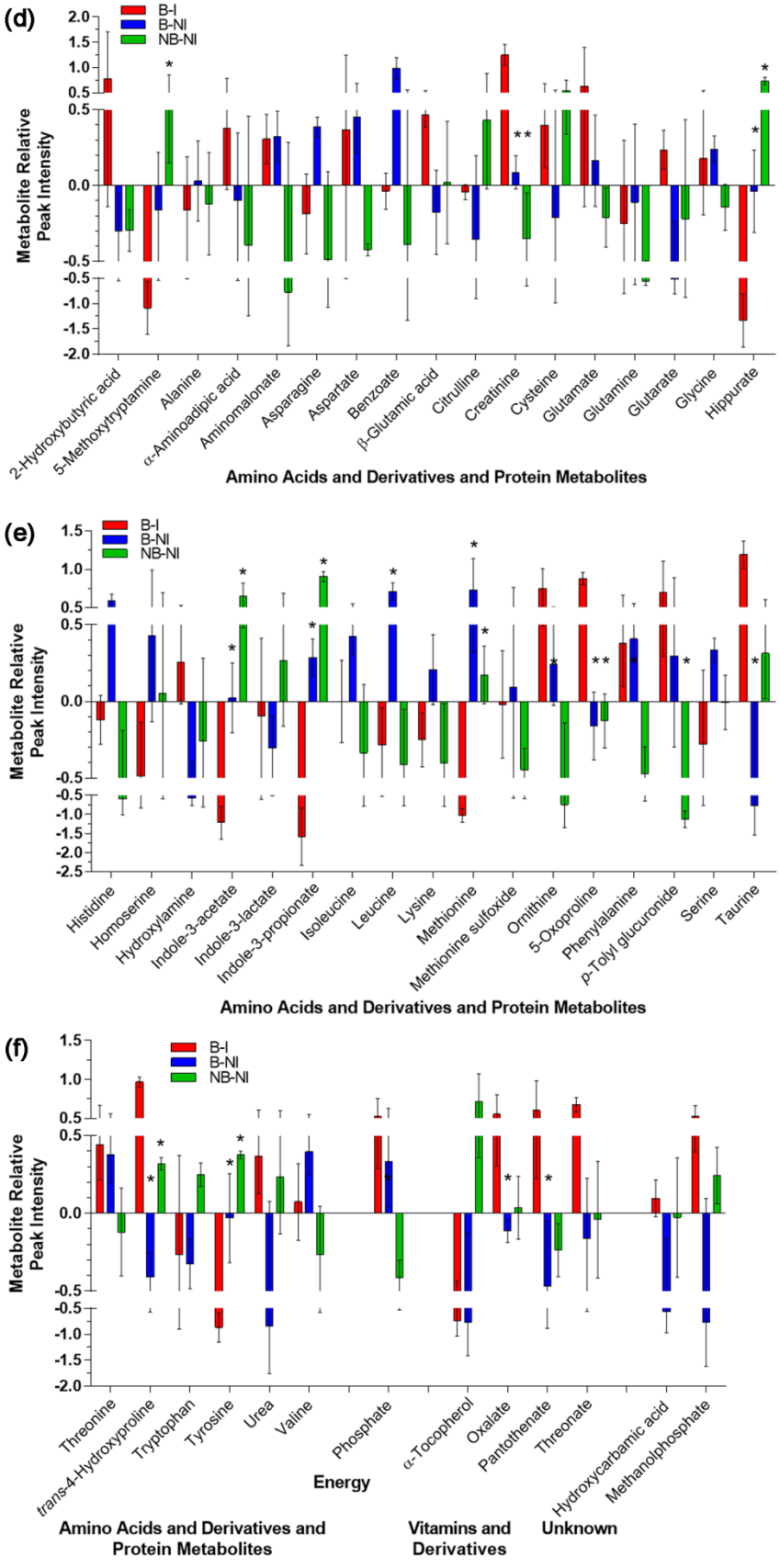
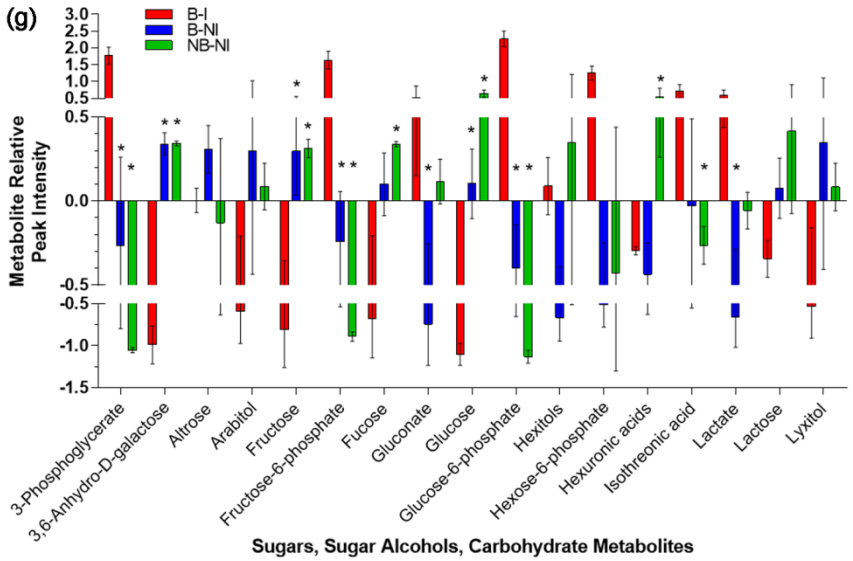
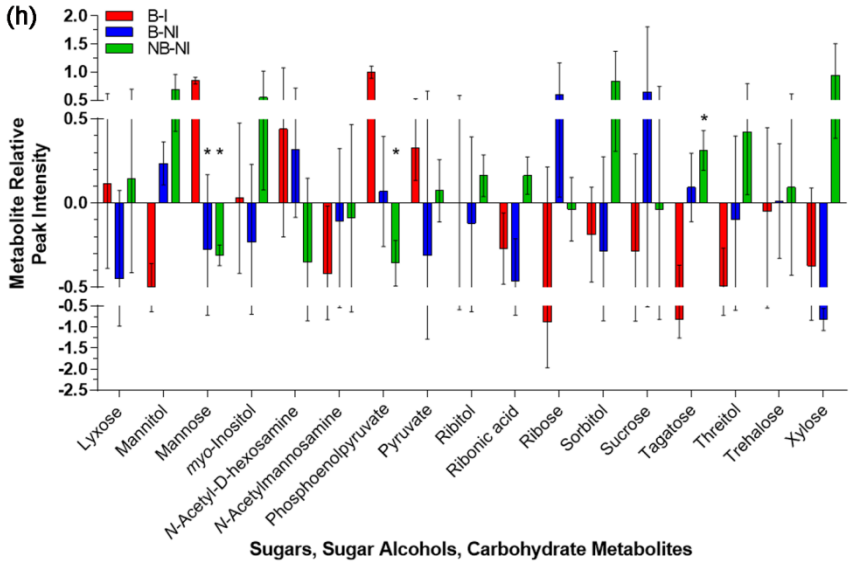
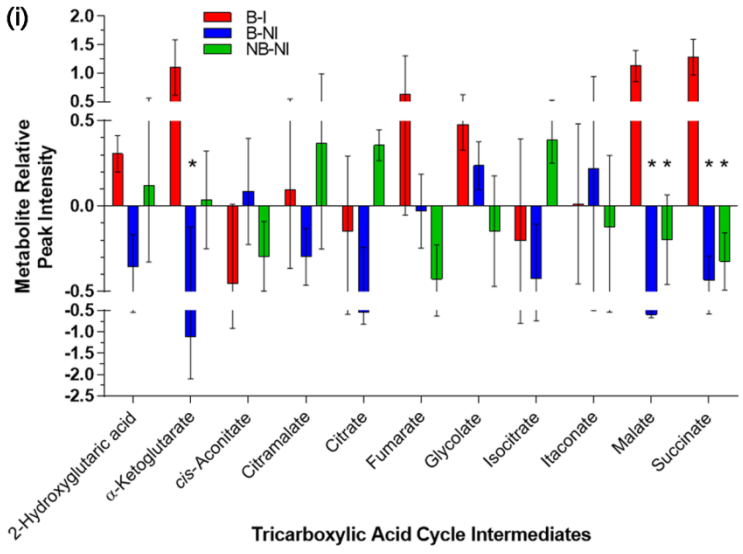
Online Resource 4: Fig. S1 Relative peak intensities of the 148 identified metabolites


(a)
B-I
B-NI
NB-NI
Metabolite Relative Peak Intensity
1-Methylinosine
Allantoic acid
Uric acid
3-Aminoisobutyric acid
3-Ureidopropionate
β-Alanine
Orotic acid
Pseudouridine
Thymidine
Thymine
Uracil
Uridine
Purine Derivatives
Pyrimidines and Derivatives
(b)
B-I
B-NI
NB-NI
Metabolite Relative Peak Intensity
1-Monoolein
3,4-Hydroxybutyric acid
3-Hydroxybutyric acid
4-Hydroxybutyric acid
Arachidic acid
Arachidonic acid
β-Glycerolphosphate
Butane-2,3-diol
Capric acid
Cholesterol
Citraconic acid
Dodecanol
Ethanolamine
Glycerol-3-galactoside
Fatty Acids and Lipid Metabolites
(c)
B-I
B-NI
NB-NI
Metabolite Relative Peak Intensity
Glyceric acid
Glycerol
Glycerol-1-phosphate
Lauric acid
Linoleic acid
Myristic acid
Nonadecanoic acid
Octadecanol
Oleic acid
Palmitic acid
Palmitoleic acid
Pelargonic acid
Stearic acid
Fatty Acids and Lipid Metabolites


(d)
B-I
B-NI
NB-NI
Metabolite Relative Peak Intensity
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
-1.5
-2.0
2-Hydroxybutyric acid
5-Methoxytryptamine
Alanine
α-Aminoadipic acid
Aminomalonate
Asparagine
Aspartate
Benzoate
β-Glutamic acid
Citrulline
Creatinine
Cysteine
Glutamate
Glutamine
Glutarate
Glycine
Hippurate
Amino Acids and Derivatives and Protein Metabolites
(e)
B-I
B-NI
NB-NI
Metabolite Relative Peak Intensity
1.5
1.0
0.5
0.0
-0.5
-1.0
-1.5
-2.0
-2.5
Histidine
Homoserine
Hydroxylamine
Indole-3-acetate
Indole-3-lactate
Indole-3-propionate
Isoleucine
Leucine
Lysine
Methionine
Methionine sulfoxide
Ornithine
5-Oxoproline
Phenylalanine
p-Tolyl glucuronide
Serine
Taurine
Amino Acids and Derivatives and Protein Metabolites
(f)
B-I
B-NI
NB-NI
Metabolite Relative Peak Intensity
1.5
1.0
0.5
0.0
-0.5
-1.0
-1.5
-2.0
Threonine
trans-4-Hydroxyproline
Tryptophan
Tyrosine
Urea
Valine
Phosphate
α-Tocopherol
Oxalate
Pantothenate
Threonate
Hydroxycarbamic acid
Methanolphosphate
Energy
Amino Acids and Derivatives and Protein Metabolites
Vitamins and Derivatives
Unknown


(g)
B-I
B-NI
NB-NI
Metabolite Relative Peak Intensity
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
-1.5
3-Phosphoglycerate
3,6-Anhydro-D-galactose
Altrose
Arabitol
Fructose
Fructose-6-phosphate
Fucose
Gluconate
Glucose
Glucose-6-phosphate
Hexitols
Hexose-6-phosphate
Hexuronic acids
Isothreonic acid
Lactate
Lactose
Lyxitol
Sugars, Sugar Alcohols, Carbohydrate Metabolites


(h)
B-I
B-NI
NB-NI
Metabolite Relative Peak Intensity
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
-1.5
-2.0
-2.5
Lyxose
Mannitol
Mannose
myo-Inositol
N-Acetyl-D-hexosamine
N-Acetylmannosamine
Phosphoenolpyruvate
Pyruvate
Ribitol
Ribonic acid
Ribose
Sorbitol
Sucrose
Tagatose
Threitol
Trehalose
Xylose
Sugars, Sugar Alcohols, Carbohydrate Metabolites


(i)
B-I
B-NI
NB-NI
Metabolite Relative Peak Intensity
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
-1.5
-2.0
-2.5
2-Hydroxyglutaric acid
α-Ketoglutarate
cis-Aconitate
Citramalate
Citrate
Fumarate
Glycolate
Isocitrate
Itaconate
Malate
Succinate
Tricarboxylic Acid Cycle Intermediates

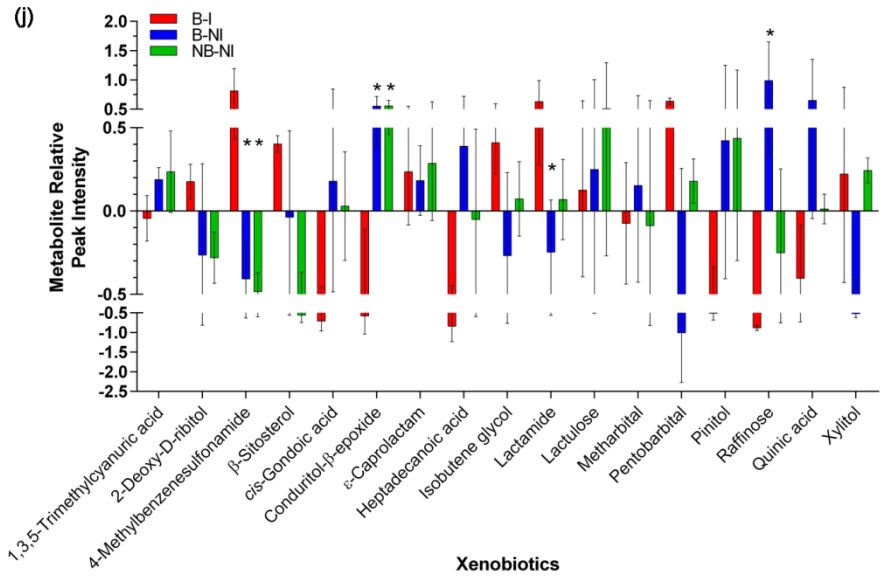


Fig. S1 Relative peak intensities of the 148 identified metabolites. Peak intensities of the identified metabolites were normalized using vector and median normalization methods. Relative peak intensities were log-transformed and scaled using Pareto scaling in the MetaboAnalyst program (https://www.metaboanalyst.ca; accessed 18 Aug 2019) (Chong et al., 2018)[1]. Values shown for the thermally injured/*P. aeruginosa* infected group (B-I), the thermally injured but not infected group (B-NI), and the sham control group (NB-NI) represent means ± SEM (*n* = 3/group). Asterisk (*) represents significance of at least *P* <0.05 as determined by one-way ANOVA (all pairs) followed by Fisher's least significance difference test. **a** purine and pyrimidine derivatives; **b, c** fatty acids and lipid metabolites; **d, e, f** amino acids and protein metabolites; **f** energy, vitamins and derivatives, unknown function; **g, h** sugars, sugar alcohols, and carbohydrate metabolites; **i** tricarboxylic acid cycle intermediates; **j** xenobiotics

[1]Chong, J., Soufan, O., Li, C., Caraus, I., Li, S., Bourque, G., et al. (2018). MetaboAnalyst 4.0: towards more transparent and integrative metabolomics analysis. *Nucleic Acids Res*, 46(W1), W486-W494. doi:10.1093/nar/gky310.