

Supplementary Table 1: List of all metabolites detected on mass spectrometry.

Metabolites					
1-Methyladenosine	Asparagine	Glucuronic acid	L-2-Aminobutyric acid	Pantothenic acid	Urate
1-Methylhistidine	Aspartic acid	Glutamic acid	Lactate	Phenylacetylglutamine	Ureidopropionic acid
1-Methylnicotinamide	Asymmetric dimethylarginine	Glutamine	Leucate	Phenylalanine	Uridine
2-Amino adipate	β -Alanine	Glutaryl carnitine	Leucine	Phenylglyoxylic acid	Valine
2-Hydroxybutyrate	Betaine	Glyceraldehyde	Linoleic acid	Phenyllactic acid	Xanthine
2-Hydroxyphenylacetate	Cadaverine	Glycerophosphocholine	Linolenic acid	Phenylpyruvic acid	Xanthurenic acid
3-Aminoisobutyrate	Caffeine	Glycine	Lysine	Pipecolic acid	Xylonic acid
3-Hydroxyanthranilic acid	Carnitine	Glycochenodeoxycholate	Malate	Proline	
3-Hydroxybutyric acid	Cholesteryl sulfate	Glycocholate	Malondialdehyde	Pseudouridine	
3-Hydroxyisovaleric acid	Choline	Glycolic acid	Mannitol	Pyroglutamic acid	
3-Hydroxyphenylacetic acid	Citrulline	Guanidinoacetate	Methionine	Pyruvate	
3-Indoxyl sulfate	Cortisol	Hippuric acid	Methionine sulfoxide	Reduced glutathione	
4-Pyridoxic acid	Cotinine	Histidine	Methylcysteine	Riboflavin	
5-Aminovaleric acid	Creatine	Homoarginine	Mevalonate	S-Adenosylmethionine	
5-Methylthioadenosine	Creatinine	Homocitrulline	MOPEG sulfate	S-Adenosylhomocysteine	
5-Methyluridine	Cystathionine	Hydrocinnamic acid	Myristic acid	Serine	
6-Methyladenosine	Cysteine-S-sulfate	Hydroxyproline	N-Acetyl-L-alanine	Sorbitol	
7-Methylguanine	Cysteinylglycine	Hypotaurine	N-Acetyl-L-aspartate	Succinate	
Acetylcarnitine	Cystine	Hypoxanthine	N-Acetyl-L-glutamic acid	Succinylcarnitine	
Adenine	Cytidine	Indole-3-acetic acid	N-Acetyl glycine	Sucrose	
Adenosine	Deoxycarnitine	Indole-3-lactate	N-Acetylneuraminate	Taurine	
Alanine	Deoxycholic acid	Indole-3-propionate	N-Formyl-L-methionine	Theophylline	
Allantoin	Dihydrouracil	Inosine	N ₂ ,N ₂ -Dimethylguanosine	Thiamine	
α -Hydroxyglutarate	Dimethylglycine	Inositol	N ₆ -Acetyl-L-lysine	Threonine	
α -Ketoglutaric acid	Erythronic acid	Isoleucine	N ₆ ,N ₆ ,N ₆ -Trimethyl-L-lysine	Thyroxine	
α -Tocopherol	Ethanolamine	Isovaleric acid	Niacinamide	Trigonelline	
AMP	Ethylmalonic acid	Isovaleryl carnitine	O-Phosphoethanolamine	Trimethylamine N-oxide	
Arabitol	FAD	Isovalerylglycine	Ornithine	Tryptophan	
Arachidonate	Gluconolactone	Kynurenic acid	Oxidized glutathione	Tyrosine	
Arginine	Glucose	Kynurenine	Palmitic acid	Uracil	

Supplementary Table 2: Evaluation of PLS-DA models comparing injury outcome groups using cross-validation and permutation tests.

	Time Point	Cross Validation		Permutation <i>p</i> value
		R ²	Q ²	
CCI/Death vs. Rapid Recovery	Hour 12	0.35	0.01	> 0.05
	Day 1	0.62	0.33	< 0.05
	Day 4	0.64	0.43	< 0.01
	Day 7	0.74	0.57	< 0.001

Supplementary Table 3: Metabolites with variable importance in projection (VIP) score > 2 for each PLS-DA comparing injury outcome groups.

	Hour 12	Day 1	Day 4	Day 7
CCI/Death vs. Rapid Recovery	Succinylcarnitine		Sucrose	Glucuronic acid
	Phenylacetylglutamine	Phenylacetylglutamine	Phenylacetylglutamine	Phenylglyoxylic acid
	MOPEG Sulfate	Hippuric acid	Trimethylamine N-oxide	Phenylacetylglutamine
	Glycochenodeoxycholate	1-Methylnicotinamide	4-Pyridoxic acid	2-Hydroxyphenylacetate
	Trimethylamine N-oxide	Trimethylamine N-oxide	Hippuric acid	Isovalerylglycine
	3-Indoxyl sulfate	Succinylcarnitine	MOPEG Sulfate	Trimethylamine N-oxide
	Glucuronic acid	3-Indoxyl sulfate	3-Hydroxybutyric acid	Indole-3-propionate
	Xanthine	Riboflavin	Indole-3-acetic acid	Pantothenic acid
	AMP	Kynurenic acid	3-Indoxyl sulfate	Cystathionine
	4-Pyridoxic acid	Cystathionine	Glucuronic acid	MOPEG Sulfate
			2-Hydroxyphenylacetate	
			Succinylcarnitine	
			Phenyllactic acid	