

Supplementary Figures

Figure S1. Typical 600 MHz high-resolution ^1H nuclear magnetic resonance (NMR) urinary spectra from control BALB/c mouse

Figure S2. Matching the gut microbial composition and urine metabolite profile by accounting one time-point lag in the latter samples

Figure S1

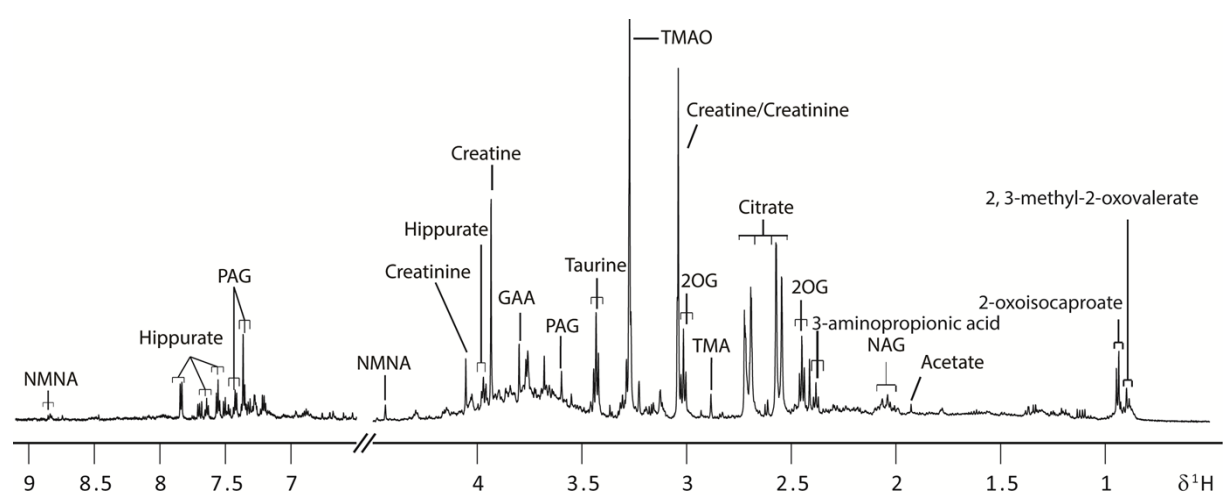


Figure S2

Urine		Stool	
Day 1		Day 1	
Day 2	←	Day 2	
Day 3	←	Day 3	
Day 8	←	Day 8	
Day 15	←	Day 15	

Supplementary table

Table S1. Urinary metabolites found to be altered between time points based on O-PLS-DA models and permutation tests.

Metabolites	Chemical shifts, ppm (multiplicity)	Time points									
		D8 vs D1 ($R^2X=$ 33.8%; $Q^2Y=87.8\%$)	D8 vs D15 ($R^2X=$ 31.3%; $Q^2Y=79.0\%$)	D1 vs D2 ($R^2X=$ 36.0%; $Q^2Y=62.6\%$)	D1 vs D3 ($R^2X=$ 31.8%; $Q^2Y=69.7\%$)	D1 vs D15 ($R^2X=$ 36.0%; $Q^2Y=71.0\%$)	D2 vs D3 ($R^2X=$ 18.1%; $Q^2Y=1.4\%$)	D2 vs D8 ($R^2X=$ 28.7%; $Q^2Y=88.5\%$)	D2 vs D15 ($R^2X=$ 21.3%; $Q^2Y=57.4\%$)	D3 vs D8 ($R^2X=$ 27.6%; $Q^2Y=81.5\%$)	D3 vs D15 ($R^2X=$ 22.7%; $Q^2Y=61.8\%$)
2,3-dihydroxybutyrate	1.24 (d)	+	+					-	-	-	
2-oxoglutarate	2.45 (t), 3.01 (t)	-	-			+	+	+		+	
Acetate	1.92 (s)	-	-					+		+	
α -hydroxy <i>N</i> -valerate	0.92 (t), 1.64 (m)	+	+							-	
Arginine	1.63(m), 1.89(m)	+	+					-		-	
Citrate	2.55 (d), 2.70 (d)	-	-			+		+	+	+	
Creatine	3.04 (s), 3.93 (s)			+	+			-	-	-	-
D-3-hydroxybutyrate	1.20 (d)	+	+					-	-	-	
Dimethylglycine	2.92 (s)	-		+	+						
Formate	8.45 (s)	-						+	+	+	
Fumarate	6.53 (s)	-						-		-	
Guanidinoacetate	3.80 (s)	-	-	+							
Hippurate	3.98 (d), 7.54 (t), 7.64 (t), 7.84 (d)	-	-		-			+		+	
<i>N</i> -acetyls of glycoproteins	2.01 (s)	+	+					-		-	
<i>N</i> -methyl nicotinate	4.44 (s), 8.84 (t), 9.12 (s)	-	-					+		+	
Phenylacetylglutamine	7.43(m), 7.37(m), 3.75(d), 3.68(s)	+		+				-	-	-	
Pyruvate	2.41 (s)	-	-		+	+		+		+	
Sarcosine	3.60 (s)	-	-					+		+	
Succinate	2.35 (s)	+	+					-		-	
Taurine	3.23 (t), 3.43 (t)	+	+			-		-	-	-	
Trimethylamine	2.89 (s)	+			-	-					
Trimethylamine <i>N</i> -oxide	3.27 (s)	+		-	-	-		-	-	-	-
Tryptophan	7.21 (t), 7.29 (t), 7.72 (d)	+				-					

Footnote: All metabolites were significant at the level of $p < 0.01$ calculated using permutation test between each pair of time points; s, singlet; d, doublet; t, triplet; m, multiplets; +, relatively higher in the first group and vice versa. Key: D1, day 1; D2, day 2; D3, day 3; D8, day 8; D15, day 15.

