

SUPPLEMENTARY TABLE 1. Multiple reaction monitoring precursor ion and product ion transitions for liquid chromatography-mass spectrometry/mass spectrometry analysis of 11 targeted urinary metabolites. Deuterated internal standards were used for hippuric acid (hippuric acid-d5) and indoxyl sulfate (indoxyl sulfate-d4).

Metabolite	Precursor		
	MW	Ion	Product Ion
Name	(g/mol)	(m/z)	(m/z)
Indole-3-propionic acid	189.2	188.2	116.2
Indoxyl sulfate	251.3	212.2	132.2
Phenylpropionylglycine	207.1	206.2	74.2
Cinnamoylglycine	205.1	204.2	160.2
Enterolactone	298.3	297.4	253.3
Enterodiol	302.4	301.4	253.3
3,4 Dihydroxyphenylacetic acid	168.2	167.1	123.2
N-Acetyl-tryptophan	246.3	245.3	203.2
Taurine	125.1	124.1	80.1
D-L Tyrosine	181.2	180.2	119.2
Hippuric acid	179.2	178.2	134.2
Hippuric acid-d ₅	184.2	183.1	139.2
Indoxyl sulfate-d ₄	217.2	216.2	136.2

m/z, mass/charge.