Supporting Information

UPLC-TQ-MS analysis

Each urine sample was analyzed using an ACQUITY UPLC system (Waters, Milford, MA, USA). The separation was carried out on an ACQUITY UPLC HSS T3 column (1.8 μm, 2.1×50 mm; Waters Corp., Milford, MA, USA) maintained at 30 °C. A 5 μL sample during each injection was eluted with a mixture of 0.1% formic acid in water (A) and acetonitrile (B). The gradient program was as follows: 0-2 min, 1% B-1% B; 2-8 min, 1% B-30% B; 8-10 min, 30% B-100% B. The flow rates were 0.3 mL min^{-1} at positive ion mode and 0.4 mL min^{-1} at negative ion mode. Mass spectrometric detection was carried out on Xevo TQ mass spectrometer (Waters, Milford, MA, USA) with an electrospray ionization (ESI) source. Quantification analysis was performed in multiple reaction monitoring (MRM). The following settings were used for MRM: capillary voltage 3.0 kV (+) and 2.0 KV (-); source temperature 350 °C; cone gas flow 50 L h^{-1}; desolvation gas flow 800 L h^{-1}; cone and collision energy are presented in Table S1. N,N-Dimethyl-L-phenylalanin was selected as the internal standard (IS) of the analysis. Data were collected and analyzed by using Masslynx V4.1 software (Waters, USA). The Regression data and LOQs of uric acid and creatinine were shown in Table S2.

Table S1 Precursor/product ion pairs and parameters for MRM of uric acid and creatinine.

Compounds	Mode	RT (min)	Precursor ion→product ion (*m/z*)	Cone voltage (V)	Collision energy (eV)
Creatinine	+	0.53	114.15→44.10	20	14
IS	+	4.18	194.21→148.16	22	16
Uric acid	-	0.79	167.08→96.06	28	18
IS	-	3.68	192.21→146.94	22	12

Table S2 Regression data and LOQs of uric acid and creatinine.

Compounds	Linear regression equations	Correlation coefficients (r)	Linear range (μmol/L)	LOQ (μmol/L)
Creatinine	Y=0.028555X+0.289891	0.9956	0.05-300	0.015
Uric acid	Y=0.189152X+0.001347	0.9980	0.01-300	0.0008

Table S3 Identification results of potential biomarkers.

Compounds	t_R (min)	*m/z*	MS/MS
Indole-3-carboxylic acid*	4.30	162.06	91.04
Xanthurenic acid*	1.40	206.04	160.04
Hippuric acid*	2.08	180.07	105.05
			77.02
Kynurenic acid*	1.68	190.05	144.05
			116.06
Creatinine*	0.41	114.07	44.10
3-Indole carboxylic acid glucuronide	2.24	338.09	162.06
Indoxyl sulfate*	1.94	212.00	132.05
			79.96
Citric acid	0.48	191.02	111.01
Azelaic acid	5.17	187.10	125.10
			96.78
Uric acid*	0.46	167.02	124.02
			96.02
			69.01
4-(2-Aminophenyl)-2,4-dioxobutanoic acid	2.00	206.05	132.05
Suberic acid*	3.74	173.08	129.09
			111.08
Sebacic acid*	3.22	201.1140	139.12
Fumaric acid	0.44	115.00	71.10
Allantoin*	0.39	157.04	113.93
			96.93
Inosine*	0.54	267.07	135.03
N-Acetylvaline	1.59	158.08	114.09
5,6-Dihydroxyindole	0.77	148.04	120.05

* Confirmed by standards