

Data S1. Materials and methods

Reagents, materials and instruments. Acetonitrile (Sigma-Aldrich; Merck KGaA); formic acid (ROE Corporation); pure water (Hangzhou Wahaha Group Co., Ltd.); Waters Acquity Ultra Performance Liquid Chromatography (UPLC) system (Waters Corporation); Acquity UPLC BEH C18 chromatographic column (Waters Corporation).

Data acquisition was performed on a UPLC quadrupole time-of-flight mass spectrometry (Q-TOF/MS) system (Waters Corporation). UPLC analysis was performed in a Waters Acquity UPLC system. Urine samples (10 μ l) were injected into an Acquity UPLC BEH C18 column (2.1x100 mm; 1.7 μ m). The column temperature was set at 45°C, and the flow rate was 0.3 ml/min. The gradient system consisted of 0.1% formic acid in water in mobile phase A and 0.1% formic acid in acetonitrile in mobile phase B (0-8.5 min, A, 99-75%; 8.5-11 min, A, 75-50%; 11-13 min, A, 50-99%; 13-15 min, A, 99%).

MS was performed on a Waters Micro mass Q-TOF micro Synapt High Definition Mass Spectrometer (Waters Corporation). Electrospray ionization (ESI) source was used

for mass spectrometric detection in positive ionization mode. The MS analysis parameters were as follows: Capillary voltage, 3.0 kV; drying gas temperature, 325°C; drying gas flow, 0.26 ml/min; desolvation gas flow 700 l/h; source temperature, 120°C; desolvation temperature, 450°C; and cone gas flow, 50 l/h. The reference ion $[M + H]^+ = 556.2771$ was used to ensure accuracy in the spectral acquisition, and the quadrupole scan range was m/z 50-1,000 Da.

Methodological investigation. Before sample UPLC-Q-TOF/MS analysis, the QC samples were injected to validate the experiments. A QC sample was injected six times consecutively for instrument precision experiment. For the method repeatability experiment, six QC samples were prepared in parallel, and continuous injection analysis was performed. The same QC sample solutions were analyzed at 0, 6, 12, 18 and 24 h for the sample stability test. In all validation experiments, 20 chromatographic peaks were selected randomly to calculate the relative standard deviation (RSD) values of the areas and the retention time of these peaks.

Table SI. Biochemical indicators in the HC group.

Parameter	HC, n=28
TC, mmol/l	4.90 (4.42,5.07)
TG, mmol/l	1.07±0.36
HDL-C, mmol/l	1.36±0.26
LDL-C, mmol/l	2.94 (2.47,3.17)
FBG, mmol/l	4.96±0.44
Cr, μ mol/l	61.86±14.41
BUN, mmol/l	4.25 (3.93,5.58)
UA, μ mol/l	261.75±58.09

Data are expressed as the mean \pm SD for normally distributed variables or as the median (interquartile range) when normality was not tenable. HC, healthy control; TC, total cholesterol; TG, triglyceride; HDL-C, high density lipoprotein cholesterol; LDL-C, low density lipoprotein cholesterol; FBG, fasting blood glucose; Cr, creatinine; BUN, blood urea nitrogen; UA, uric acid.

Table SII. Treatments administered to patients with unstable angina.

Category	Drug	Frequency (%)
Antiplatelet	Aspirin	23 (82.14)
	Clopidogrel	10 (35.71)
Statins	Atorvastatin	12 (42.86)
	Rosuvastatin	8 (28.57)
	Pravastatin	2 (7.14)
	Lovastatin	1 (3.57)
Beta blocker	Metoprolol	15 (53.57)
Nitrates	Isosorbide dinitrate	10 (35.71)
Energy metabolism	Trimetazidine	5 (17.86)
Calcium channel blockers	Diltiazem	2 (7.14)
	Amlodipine	2 (7.14)
	Felodipine	1 (3.57)
	Nifedipine	1 (3.57)
Angiotensin II reuptake blockers	Valsartan	3 (10.71)
	Irbesartan	1 (3.57)
Angiotensin-converting enzyme inhibitor	Fosinopril	2 (7.14)
	Benazepril	2 (7.14)
	Perindopril	1 (3.57)
Potassium channel opener	Nicorandil	1 (3.57)