

Table 1. Clinical characteristics of the severe sepsis patients

Parameter	Healthy volunteers (n = 1346)	SS Patients (n = 1282)	P value
Age, years	55.3 ± 10.2	57.2 ± 8.8	0.33
Sex (male/female)	660/686	640/642	0.72
BMI, kg/m ²	24.15 ± 1.27	25.32 ± 3.52	0.69
DBP, mmHg	75.13 ± 8.16	76.44 ± 8.21	0.49
SBP, mmHg	147.10 ± 22.31	145.09 ± 23.38	0.66
Serum FBG, mmol/L	5.7 ± 1.3	5.9 ± 1.5	0.19
Serum TG, mmol/L	2.5 ± 0.4	1.8 ± 0.3	0.04
Serum TC, mmol/L	4.7 ± 0.6	4.8 ± 0.7	0.53
Serum insulin, mmol/L	12.4 ± 3.7	25.9 ± 6.1	0.0042
PCT, ng/ml	10.3 ± 2.5	5.7 ± 1.6	0.0006
ISS	54.6 ± 7.2	33.5 ± 7.7	0.0008

Note: A-AP, A-amyloid protein; BMI, body mass index; DBP, diastolic blood pressure; FBG, fasting (2 hours postprandial) blood glucose; SBP, systolic blood pressure; TC, total cholesterol; TG, triglycerides; ISS: Injury severity score. The p values less than 0.05 were considered significant.

Table S2. Information of SS biomarkers detected by UPLC-Q-TOF/MS in positive ion mode

No	VIP	Rt	m/z	Formula	Mass Error (ppm)	Description	Anova (p)	Trend
1	14.34	3.51	190.0567	C10H7NO3	-2.80	Kynurenic acid	0.0002	↓
2	14.05	4.09	180.0734	C9H9NO3	-2.62	Hippuric acid	0.0003	↑
3	11.52	4.65	76.0469	C2H5NO2	-1.08	Glycine	0.0008	↓
4	11.11	0.86	259.0974	C10H14N2O6	-0.70	3-Methyluridine	0.0004	↑
5	11.07	7.27	164.0480	C5H9NO3S	-3.81	Acetylcysteine	0.0004	↑

Table S3. ROC curve analysis of potential biomarkers in SS detected by UPLC/MS

No	Metabolite	AUC	Sensitivity (%)	Specificity (%)
1	Kynurenic acid	0.985	96.2	97.0
2	Hippuric acid	0.905	93.1	87.2
3	Glycine	0.963	83.7	89.3
4	3-Methyluridine	0.861	90.3	89.7
5	Acetylcysteine	0.811	80.2	85.5