Table S1. Clinical characteristics of the severe sepsis patients

Parameter	Healthy volunteers	SS Patients	P value
Age, years	55.3 ± 10.2	57.2 ± 8.8	0.33
Sex (male/female)	360/222	340/206	0.72
BMI, kg/m2	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-MS in negative ion mode

No	VIP	Rt	m/z	Compound ID	Formula	Mass Error (ppm)	Description	Anova (p)	Trend
1	15.84	2.78	165.0546	HMDB00748	C9H10O3	-1.54	3-Phenyllactic acid	0.0007	↑
2	27.83	1.62	211.0635	HMDB00913	C10H12O5	1.05	Vanillactic acid	0.0021	↓
3	27.53	1.28	194.0449	HMDB06116	C9H9NO4	-1.92	3-Hydroxyhippuric acid	0.0002	↑
4	23.21	2.69	129.0556	HMDB00695	C6H10O3	-0.62	Ketoleucine	0.0035	↓
5	18.16	1.57	357.1306	HMDB01069	C16H18N6O4	-0.95	2-Phenylaminoadenosine	0.0411	↓
6	11.19	3.80	210.0796	HMDB01434	C10H13NO4	0.65	3-Methoxytyrosine	0.0032	↑

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

No	Metabolite	AUC	Sensitivity (%)	Specificity (%)
1	3-Phenyllactic acid	0.993	98.2	99.3
2	Vanillactic acid	0.885	92.1	91.8
3	3-Hydroxyhippuric acid	0.981	63.2	82.4
4	Ketoleucine	0.876	93.7	92.1
5	2-Phenylaminoadenosine	0.885	81.2	97.3
6	3-Methoxytyrosine	0.802	81.3	87.2