

Table S1. Demographic and baseline characteristics of the subjects enrolled in the study.

Parameter	Patients (n = 106)	Healthy volunteers (n = 101)	P value #
Age, years	58±5	56±4	0.77
Sex (male/female)	55/51	51/50	0.83
Days in the ICU	7±2	none	0.00
Body mass index (kg/m ²)	23.35±5.19	24.76±6.34	0.76
APACHE II	16.0±2.7	6.70±2.01	0.02
SOFA-24h	7.29±1.34	2.06±0.39	0.01
Hemoglobin (g/dl)	11.17±4.04	14.28±3.70	0.11
Leukocytes (x10 ⁹ /l)	14.06±1.38	19.20±4.63	0.04
Platelets (x10 ⁹ /l)	187.0±34.27	280.4±68.24	0.00
PCR (mg/l)	187±38	267±49	0.01
PCT (ng/ml)	3.2±0.4	1.4±0.1	0.01
Urea (mg/dl)	66±12	51±10	0.06

Note: ICU intensive care unit, APACHE II Acute Physiology and Chronic Health Evaluation II, SOFA Sequential Organ Failure Assessment, PCT procalcitonin, PCR reactive C protein. *p values <0.05.

Table S2. Information of SIALI marker metabolites detected by high-resolution mass spectrometry

No	Rt (min)	m/z	Compound ID	Formula	Ppm	Description	p	VIP	Trend	AUC	Sensitivity	Specificity
1	2.93	248.1129	HMDB02095	C ₁₀ H ₁₇ NO ₆	0.13	Malonylcarnitine	0.0000	16.33	↑	0.995	97.0	96.3
2	2.11	147.0770	HMDB03423	C ₅ H ₁₀ N ₂ O ₃	0.87	D-Glutamine	0.0000	17.18	↑	0.987	96.9	97.5
3	4.43	212.0901	HMDB01434	C ₁₀ H ₁₃ NO ₄	-0.79	3-Methoxytyrosine	0.0000	18.17	↑	0.961	85.8	96.2
4	7.40	225.0861	HMDB12819	C ₁₀ H ₁₂ N ₂ O ₄	-0.91	5-Hydroxykynurenine	0.0000	19.82	↑	0.874	83.1	87.2
5	4.55	151.0619	HMDB13141	C ₆ H ₆ N ₄ O	1.20	1-Methylhypoxanthine	0.0000	19.26	↓	0.854	86.0	84.6
6	1.67	118.0865	HMDB00883	C ₅ H ₁₁ NO ₂	1.08	L-Valine	0.0000	30.12	↓	0.833	85.8	82.5

Note: a, all compounds are verified with an authentic standard.