Table S1. Characterization of chemical components in XJDHT by UPLC–QTOF–MS

No.	t_R (min)	Molecular ion MS^1	Error (ppm)	Fragment ions in negative mode MS^2	Molecular formula	Identity
1	0.84	341.1089 $[M-H]^-$	1.46	221 $[M-H-C_4H_8O_4]^-$, 179 $[M-H-C_6H_{10}O_5]^-$, 161 $[M-H-C_6H_{10}O_5-H_2O]^-$,	$C_{12}H_{22}O_{11}$	Gentiobiose
2	0.9	493.1198 $[M-H]^-$	0.81	313 $[M-H-Glc]^-$, 169 [Gallic acid-H]$^-$	$C_{19}H_{26}O_{15}$	Galloylsucrose
3	1.13	407.1199 $[M-H]^-$	2.21	199 $[M-H-Glc]^-$, 169 $[M-H-Glc-CH_2O]^-$	$C_{15}H_{22}O_{10}$	Catalpol
4	1.62	169.0147 $[M-H]^-$	2.95	125 $[M-H-CO_2]^-$,	$C_7H_6O_5$	Gallic acid
5	1.66	345.1556 $[M-H]^-$	2.02	301 $[M-H-CO_2]^-$, 283 $[M-H-CO_2-H_2O]^-$	$C_{16}H_{26}O_8$	Rehmannioside D
6	2.97	343.1399 $[M+HCOO]^-$	1.74	181 $[M-H-Glc]^-$, 151 $[M-H-Glc-CH_2O]^-$	$C_{16}H_{24}O_8$	Mudanpioside F
7	3.65	495.1509 $[M-H]^-$	1.21	465 $[M-H-CH_2O]^-$, 195 $[M-H-C_6H_{10}O_5-$ hydrobenzoyl$]^-$, 137 [Hydroxybenzoic acid-H]$^-$	$C_{23}H_{28}O_{12}$	Oxypaeoniflorin
8	3.67	289.0722 $[M-H]^-$	3.45	245 $[M-H-CO_2]^-$, 179 $[M-H-C_6H_6O_2]^-$, 165 $[M-H-C_7H_8O_2]^-$	$C_{15}H_{14}O_6$	Catechin
9	3.95	525.1618 $[M-H]^-$	1.90	495 $[M-H-CH_2O]^-$, 429 $[M-H-CH_2O-CH_2O-2H_2O]^-$	$C_{24}H_{30}O_{13}$	Mudanpioside E
10	4.22	345.1555$[M-H]^-$	1.73	495 $[M-H-CO_2]^-$	$C_{16}H_{26}O_8$	Rehmapicroside

11	4.40	525.1617[M+HCOO]$^-$	1.71	479 [M-H]$^-$, 449 [M-H-CH_2O]$^-$, 121 [Benzoic acid-H]$^-$	$C_{23}H_{28}O_{11}$	Albiflorin
12	4.53	525.1615 [M+HCOO]$^-$	1.33	479.1559 [M-H]$^-$, 449 [M-H-CH_2O]$^-$, 357 [M-H-benzoyl]$^-$, 121 [Benzoic acid-H]$^-$	$C_{23}H_{28}O_{11}$	Paeoniflorin
13	4.64	495.1508 [M-H]$^-$	1.00	465 [M-H-CH_2O]$^-$, 195 [M-H-$C_6H_{10}O_5$-hydrobenzoyl]$^-$, 137 [Hydroxybenzoic acid-H]$^-$	$C_{23}H_{28}O_{12}$	Oxypaeoniflorin isomer
14	4.73	813.2826 [M-H]$^-$	1.11	637 [M-H-$C_{10}H_8O_3$]$^-$, 619 [M-H-$C_{10}H_8O_3$-H_2O]$^-$, 193 [Ferulic acid-H]$^-$, 175 [Ferulic acid-H-H_2O]$^-$	$C_{37}H_{50}O_{20}$	Jionoside B1
15	4.74	623.1983 [M-H]$^-$	1.12	461 [M-H-Glc]$^-$, 179 [Glucose-H]$^-$, 161 [Glucose-H_2O]$^-$	$C_{29}H_{36}O_{15}$	Verbascoside
16	4.88	623.1979 [M-H]$^-$	0.48	461 [M-H-Glc]$^-$, 179 [Glucose-H]$^-$, 161 [Glucose-H-H_2O]$^-$	$C_{29}H_{36}O_{15}$	Isoacteoside
17	5.44	629.1879 [M+HCOO]$^-$	1.43	583 [M-H]$^-$, 553 [M-H-CH_2O]$^-$, 121 [Benzoic acid-H]$^-$	$C_{30}H_{32}O_{12}$	Benzoylalbiflorin
18	6.49	813.2829 [M-H]$^-$	1.47	637 [M-H-$C_{10}H_8O_3$]$^-$, 619 [M-H-$C_{10}H_8O_3$-H_2O]$^-$, 193 [Ferulic acid-H]$^-$, 175 [Ferulic acid-H-H_2O]$^-$	$C_{37}H_{50}O_{20}$	Jionoside B1 isomer

19	7.06	939.1124 $[M-H]^-$	2.12	769 $[M-H-C_7H_6O_5]^-$, 465 $[M-H-C_7H_6O_5-2C_7H_4O_4]^-$, 169 [Gallic acid-H]$^-$	$C_{41}H_{32}O_{26}$	Pentagalloylglucose
20	7.32	183.1964$[M-H]^-$	2.18	-	$C_9H_{10}O_3$	paeonol

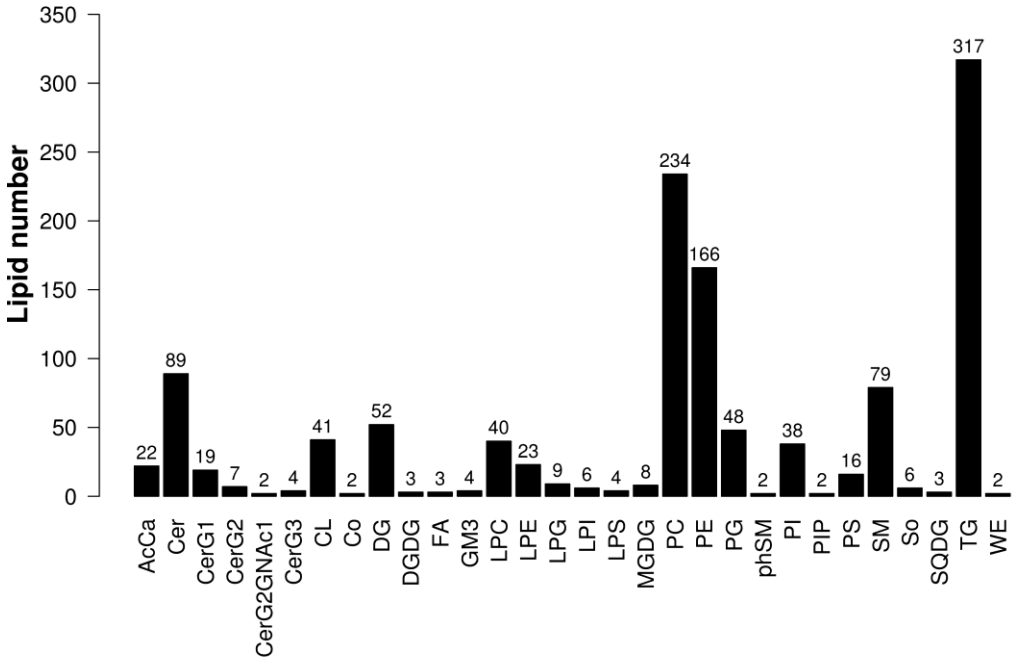

Figure S1 Lipid class and the lipid molecules identified by positive and negative ion modes

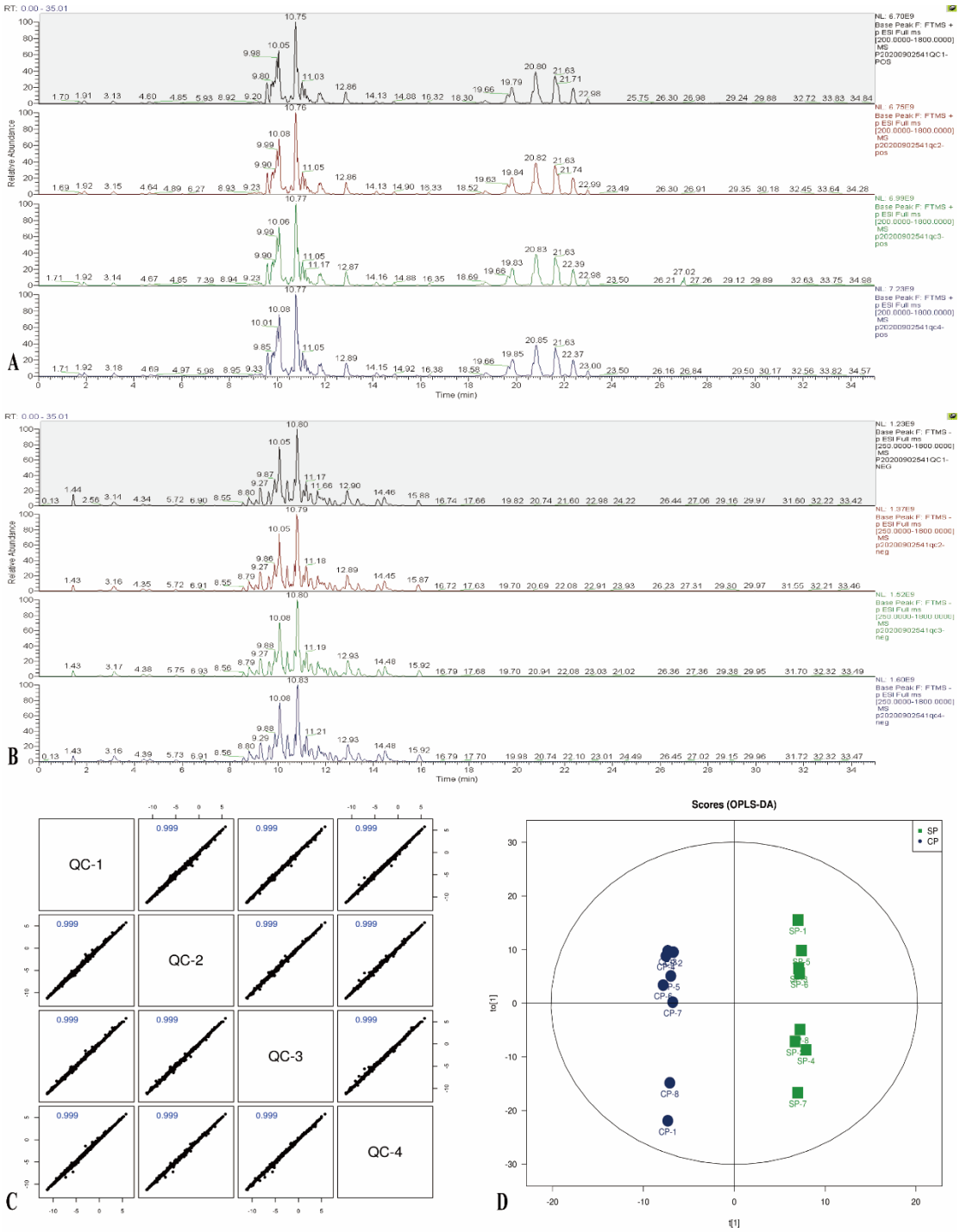

Figure S2 Experimental quality control of LC-MS/MS lipid analysis of Lung tissue.

A: The comparison base peak chromatograms (BPC) spectra of QC samples in positive-ion mode ; B： The comparison base peak chromatograms (BPC) spectra of QC samples in negative-ion mode; C: Correlation map of QC samples: The horizontal and vertical

coordinates in the figure represent each QC sample. The points in each cell represent the ions extracted by QC samples peak (metabolite), abscissa, and ordinate represent the logarithm of the signal intensity value of the ion peak. D: OPLS-DA score plot of SP-CP (The R2Y and Q2 evaluation parameters of OPLS-DA are 0.812 and 0.998 respectively).

Table S2 Differences in lipids between sepsis and Control group

No.	LipidIon	IonFormula	CalMz	RT-(min)	Fold Change	P-value	VIP	Change trend	Statistical significance
15POS	AcCa(16:0)+H	C23 H46 O4 N1	400.3421	3.05	1.52	0.022	1.02	↑	*
191POS	DG(16:0/16:1)+NH4	C35 H70 O5 N1	584.5249	11.88	0.56	0.033	1.14	↓	*
282POS	DG(16:0/22:6)+NH4	C41 H72 O5 N1	658.5405	11.42	2.42	0.007	6.03	↑	**
321POS	DG(18:0/22:4)+NH4	C43 H80 O5 N1	690.6031	13.70	1.69	0.043	1.85	↑	*
314POS	DG(18:0/22:6)+NH4	C43 H76 O5 N1	686.5718	12.49	2.10	0.008	3.15	↑	**
112POS	LPS(20:4)+H	C26 H45 O9 N1 P1	546.2826	2.23	2.17	0.004	1.59	↑	**
153POS	LPS(22:4)+H	C28 H49 O9 N1 P1	574.3139	2.61	2.39	0.008	1.08	↑	**
147POS	LPS(22:6)+H	C28 H45 O9 N1 P1	570.2826	2.13	3.28	0.003	2.01	↑	**
1402NEG	PC(14:0/14:0)+HCOO	C37 H73 O10 N1 P1	722.4978	8.68	0.26	0.000	1.52	↓	**
1543NEG	PC(16:0e/18:2)+HCOO	C43 H83 O9 N1 P1	788.5811	10.72	1.62	0.000	1.32	↑	**
1444NEG	PC(16:1/14:0)+HCOO	C39 H75 O10 N1 P1	748.5134	8.90	0.66	0.007	1.15	↓	**
1503NEG	PC(16:1/16:1)+HCOO	C41 H77 O10 N1 P1	774.5291	9.07	2.18	0.000	2.55	↑	**
1617NEG	PC(18:0p/18:2)+HCOO	C45 H85 O9 N1 P1	814.5967	10.75	2.25	0.000	1.01	↑	**

1805NEG	PC(18:1/22:6)+HCOO	C49 H83 O10 N1 P1	876.576	9.69	1.73	0.000	1.70	↑	**
460POS	PC(34:3)+H	C42 H79 O8 N1 P1	756.5538	9.21	1.93	0.002	1.83	↑	**
586POS	PC(37:6)+H	C45 H79 O8 N1 P1	792.5538	10.86	1.50	0.000	1.61	↑	**
1349NEG	PE(16:0/16:1)-H	C37 H71 O8 N1 P1	688.4923	10.23	0.29	0.000	1.54	↓	**
1337NEG	PE(32:0p)-H	C37 H73 O7 N1 P1	674.513	11.63	0.55	0.000	1.01	↓	**
638POS	PE(42:7p)+H	C47 H81 O7 N1 P1	802.5745	12.36	0.63	0.000	1.12	↓	**
1396NEG	PG(16:0/16:1)-H	C38 H72 O10 N0 P1	719.4869	9.10	0.64	0.003	1.53	↓	**
1506NEG	PG(18:0/18:1)-H	C42 H80 O10 N0 P1	775.5495	10.84	1.71	0.000	1.17	↑	**
1495NEG	PG(18:1/18:2)-H	C42 H76 O10 N0 P1	771.5182	9.35	2.62	0.000	1.41	↑	**
1774NEG	PG(22:6/22:6)-H	C50 H74 O10 N0 P1	865.5025	6.91	3.96	0.000	1.18	↑	**
1762NEG	PI(18:1/18:1)-H	C45 H82 O13 N0 P1	861.5499	9.95	1.61	0.000	1.36	↑	**
656POS	PS(16:0/22:6)+H	C44 H75 O10 N1 P1	808.5123	8.71	2.13	0.001	1.93	↑	**
811POS	PS(40:4)+H	C46 H83 O10 N1 P1	840.5749	10.99	0.53	0.004	3.31	↓	**
924POS	PS(42:1)+H	C48 H93 O10 N1 P1	874.6532	14.07	0.40	0.004	1.27	↓	**
1437NEG	SM(d16:0/18:2)+HCOO	C40 H78 O8 N2 P1	745.5501	8.85	2.55	0.033	1.60	↑	*
1448NEG	SM(d18:0/16:0)+HCOO	C40 H82 O8 N2 P1	749.5814	10.25	1.57	0.000	3.59	↑	**
1513NEG	SM(d20:0/16:0)+HCOO	C42 H86 O8 N2 P1	777.6127	11.27	1.72	0.000	2.00	↑	**
1753NEG	SM(d24:0/18:2)+HCOO	C48 H94 O8 N2 P1	857.6753	12.35	1.82	0.000	2.29	↑	**
615POS	TG(16:0/14:0/16:0)+NH4	C49 H98 O6 N1	796.7389	20.70	0.31	0.012	1.86	↓	*
729POS	TG(16:0/14:0/18:1)+NH4	C51 H100 O6 N1	822.7545	20.70	0.37	0.029	4.03	↓	*

740POS	TG(16:0/16:0/16:0)+NH4	C51 H102 O6 N1	824.7702	21.66	0.43	0.001	3.35	↓	**
848POS	TG(16:0/16:0/18:1)+NH4	C53 H104 O6 N1	850.7858	20.76	0.45	0.020	3.34	↓	*
849POS	TG(16:0/16:0/18:1)+NH4	C53 H104 O6 N1	850.7858	21.64	0.53	0.014	6.33	↓	*
858POS	TG(18:0/16:0/16:0)+NH4	C53 H106 O6 N1	852.8015	22.41	0.52	0.035	2.34	↓	*
1117POS	TG(18:0/18:1/22:4)+NH4	C61 H112 O6 N1	954.8484	21.99	1.66	0.027	1.01	↑	*
1149POS	TG(18:1/20:3/22:4)+NH4	C63 H110 O6 N1	976.8328	20.01	2.09	0.044	1.05	↑	*
1146POS	TG(20:3/18:2/22:4)+NH4	C63 H108 O6 N1	974.8171	18.89	1.61	0.045	1.02	↑	*