

Table S1 Serum metabolic biomarkers related to acute pneumonia and their change trends in different groups

No	Metabolite	Retention time (min)	Formula	Detected m/z	Mass error (ppm)	Adducts	HMDB ID	control vs Model	ZSD-H vs Model
1	Azelaic acid	21.70	C ₉ H ₁₆ O ₄	375.2020	-1.06	[2M-H]-	HMDB0000784	↑**	↑
2	Tetracosanoic acid	18.55	C ₂₄ H ₄₈ O ₂	367.3578	-0.97	[M-H]-	HMDB0002003	↑*	↑
3	LysoPA(0:0/18:2(9Z,12Z))	7.46	C ₂₁ H ₃₉ O ₇ P	433.2361	-0.01	[M-H]-	HMDB0007852	↑****	↑#
4	PC(14:0/20:2(11Z,14Z))	21.84	C ₄₂ H ₈₀ NO ₈ P	802.5573	-4.00	[M+FA-H]-	HMDB0007880	↑**	↑#
5	PC(14:0/22:5(4Z,7Z,10Z,13Z,16Z))	17.91	C ₄₄ H ₇₈ NO ₈ P	824.5430	-2.23	[M+FA-H]-	HMDB0007890	↑**	↑#
6	PC(15:0/18:2(9Z,12Z))	21.75	C ₄₁ H ₇₈ NO ₈ P	742.5356	-4.89	[M-H]-	HMDB0007940	↑**	↑###
7	10,11-dihydro-20-trihydroxy-leukotriene B ₄	6.50	C ₂₀ H ₃₄ O ₇	385.2256	6.16	[M-H]-	HMDB0012503	↑**	↑
8	PC(O-18:1(9Z)/20:4(8Z,11Z,14Z,17Z))	22.09	C ₄₆ H ₈₄ NO ₇ P	792.5884	-3.61	[M-H]-	HMDB0013432	↑**	↑###
9	TG(24:1(15Z)/20:0/24:1(15Z))	4.34	C ₇₁ H ₁₃₄ O ₆	1128.0239	7.09	[M+FA-H]-	HMDB0051981	↑**	↓
10	PA(22:0/22:2(13Z,16Z))	21.68	C ₄₇ H ₈₉ O ₈ P	811.6199	-2.85	[M-H]-	HMDB0115262	↑****	↑
11	PG(22:6(4Z,7Z,10Z,13Z,16Z,19Z)/16:0)	21.69	C ₄₄ H ₇₅ O ₁₀ P	775.4939	2.45	[M-H ₂ O-H]-	HMDB0116629	↑*	↑#

12	PA(17:0/22:6(5Z,7Z,10Z,13Z,16Z,19Z)-OH(4))	21.69	C42H71O9P	731.4627	-4.08	[M-H2O-H]-	HMDB0263549	↑*	↑
13	PGP(18:1(12Z)-O(9S,10R)/a-21:0)	17.85	C45H86O14P2	911.5465	4.92	[M-H]-	HMDB0274634	↑*	↑
14	PIP(16:0/18:3(10,12,15)-OH(9))	4.43	C43H78O17P2	909.4521	-1.56	[M-H]-	HMDB0278503	↓*	↓
15	PS(PGF1alpha/22:5(4Z,7Z,10Z,13Z,16Z))	7.84	C48H80NO13P	944.5007	-5.94	[M+Cl]-	HMDB0283389	↑*	↑
16	PC(LTE4/16:0)	16.09	C47H85N2O11PS	961.5673	8.69	[M+FA-H]-	HMDB0285930	↑*	↑
17	SM(d18:2(4E,14Z)/LTE4)	7.74	C46H82N3O9PS	882.5431	-0.64	[M-H]-	HMDB0290573	↑*	↑#
18	Trihexosylceramide (d18:1/24:1(15Z))	5.60	C60H111NO18	1116.7747	-1.84	[M+H-H2O]+	HMDB0004883	↓**	↓
19	LysoPA(0:0/18:1(9Z))	7.83	C21H41O7P	873.5199	-6.16	[2M+H]+	HMDB0007851	↑***	↑##
20	PE(18:4(6Z,9Z,12Z,15Z)/P-16:0)	17.03	C39H70NO7P	696.4982	2.85	[M+H]+	HMDB0009213	↑***	↑
21	LysoPC(16:0/0:0)	17.62	C24H50NO7P	496.3421	4.65	[M+H]+	HMDB0010382	↑*	↑#
22	MG(0:0/15:0/0:0)	5.90	C18H36O4	334.2980	8.82	[M+NH4]+	HMDB0011532	↑**	↑
23	5,6-Dihydroxyprostaglandin F1a	4.49	C20H36O7	389.2537	0.93	[M+H]+	HMDB0012109	↑***	↑
24	Nopalinic acid	7.48	C10H18N2O6	280.1507	1.52	[M+NH4]+	HMDB0029437	↑**	↑
25	TG(15:0/20:0/O-18:0)	7.82	C56H110O5	863.8509	9.59	[M+H]+	HMDB0043104	↑*	↑
26	TG(15:0/24:0/20:3(5Z,8Z,11Z))	5.94	C62H114O6	955.8770	8.59	[M+H]+	HMDB0043145	↑*	↑
27	TG(15:0/22:5(4Z,7Z,10Z,13Z,16Z)/20:2n6)	5.91	C60H102O6	936.8076	6.65	[M+NH4]+	HMDB0043614	↑*	↑

28	TG(15:0/18:4(6Z,9Z,12Z,15Z)/22:6(4Z,7Z,10Z,13Z,16Z,19Z))	7.41	C58H92O6	849.6673	-9.30	[M+H-2H2O] ⁺	HMDB0043683	↑**	↑
29	TG(21:0/i-24:0/i-16:0)	5.25	C64H124O6	971.9291	-7.52	[M+H-H2O] ⁺	HMDB0067164	↑*	↑
30	DG(i-18:0/a-25:0/0:0)	21.79	C46H90O5	723.6853	-1.10	[M+H] ⁺	HMDB0093993	↑*	↑
31	FAHFA(18:0/9-O-18:0)	14.01	C36H70O4	584.5637	4.40	[M+NH4] ⁺	HMDB0112112	↑*	↑
32	PS(18:1(11Z)/18:0)	12.30	C42H80NO10P	790.5624	3.98	[M+H] ⁺	HMDB0112388	↑*	↑#
33	LysoPA(8:0/0:0)	8.78	C11H23O7P	316.1518	-0.47	[M+NH4] ⁺	HMDB0114740	↑**	↑
34	LysoPA(a-25:0/0:0)	9.79	C28H57O7P	501.3718	2.74	[M+H-2H2O]	HMDB0114762	↑***	↑
35	PA(15:0/24:0)	5.61	C42H83O8P	1494.1756	2.17	[2M+H] ⁺	HMDB0114831	↓**	↓
36	PA(18:0/20:4(8Z,11Z,14Z,17Z))	6.68	C41H73O8P	1467.0309	-7.99	[2M+NH4] ⁺	HMDB0114885	↓*	↓
37	PA(22:2(13Z,16Z)/24:0)	5.42	C49H93O8P	858.7021	8.84	[M+NH4] ⁺	HMDB0115321	↑*	↓
38	CDP-DG(a-17:0/18:2(9Z,11Z))	7.47	C47H83N3O15P2	974.5282	1.54	[M+H-H2O] ⁺	HMDB0116098	↑*	↑##
39	PG(a-13:0/i-16:0)	16.47	C35H69O10P	698.5013	6.83	[M+NH4] ⁺	HMDB0116646	↑*	↑
40	PG(a-13:0/i-20:0)	5.60	C39H77O10P	1474.0533	-3.28	[2M+H] ⁺	HMDB0116650	↓**	↓#
41	CL(8:0/8:0/13:0/18:2(9Z,11Z))	5.11	C56H104O17P2	1093.6614	-9.21	[M+H-H2O] ⁺	HMDB0116977	↑**	↑
42	CL(10:0/18:2(9Z,11Z)/18:2(9Z,11Z)/25:0)	21.73	C80H148O17P2	1408.0019	-2.34	[M+H-2H2O] ⁺	HMDB0193969	↑**	↓
43	CL(11:0/i-18:0/18:2(9Z,11Z)/23:0)	6.48	C79H150O17P2	1456.0184	-3.95	[M+Na] ⁺	HMDB0200389	↓***	↓###

44	N-Stearoyltaurine	16.82	C20H41NO4S	392.2844	3.76	[M+H] ⁺	HMDB0240595	↑***	↑#
45	N-Stearoyl Proline	21.78	C23H43NO3	399.3569	-3.31	[M+NH4] ⁺	HMDB0241948	↑***	↑
46	N-Arachidonoyl Aspartic acid	7.65	C24H37NO5	442.2543	-5.01	[M+Na] ⁺	HMDB0241992	↑**	↑
47	Hexadecasphingosine	5.96	C16H33NO2	272.2610	9.72	[M+H] ⁺	HMDB0242181	↑**	↑
48	Aminopentol	5.94	C22H47NO5	406.3547	4.89	[M+H] ⁺	HMDB0248328	↑**	↑
49	Cholestane-3,5,6-triol	7.98	C27H48O3	438.3948	1.47	[M+NH4] ⁺	HMDB0250164	↑**	↑#
50	Glutamine glutamate aspartate	21.75	C19H27N5O15	1148.3348	0.24	[2M+NH4] ⁺	HMDB0252809	↑**	↑
51	PA(20:4(5Z,8Z,11Z,14Z)-OH(19S)/8:0)	6.34	C31H53O9P	1201.6972	3.70	[2M+H] ⁺	HMDB0266596	↓*	↓#
52	PG(20:5(7Z,9Z,11E,13E,17Z)-3OH(5,6,15)/20:4(5Z,8Z,11Z,14Z))	8.62	C46H73O13P	865.4871	1.04	[M+H] ⁺	HMDB0269977	↑**	↑#
53	PG(20:5(7Z,9Z,11E,13E,17Z)-3OH(5,6,15)/20:4(8Z,11Z,14Z,17Z))	8.72	C46H73O13P	865.4870	0.96	[M+H] ⁺	HMDB0270081	↑**	↑
54	PG(20:5(7Z,9Z,11E,13E,17Z)-3OH(5,6,15)/i-12:0)	7.42	C38H65O13P	778.4521	2.59	[M+NH4] ⁺	HMDB0271120	↑***	↑#
55	PGP(18:1(12Z)-O(9S,10R)/a-25:0)	5.24	C49H94O14P2	986.6537	8.26	[M+NH4] ⁺	HMDB0274738	↑**	↓
56	PGP(PGJ2/i-13:0)	5.52	C39H68O15P2	821.4064	7.57	[M+H-H2O] ⁺	HMDB0274922	↑**	↓
57	PGP(LTE4/i-22:0)	7.18	C51H93NO16P2S	1087.6066	3.48	[M+NH4] ⁺	HMDB0275857	↓**	↑
58	PGP(18:1(12Z)-2OH(9,10)/i-22:0)	7.05	C46H90O15P2	945.5885	6.11	[M+H] ⁺	HMDB0275877	↑**	↑###
59	PI(18:1(12Z)-2OH(9,10)/16:1(9Z))	7.83	C43H79O15P	867.5245	1.84	[M+H] ⁺	HMDB0276187	↑***	↑

60	PI(20:4(5Z,8Z,11Z,14Z)-OH(20)/20:1(11Z))	8.71	C49H85O14P	911.567 7	3.58	M+H- H2O]+	HMDB02770 72	↑**	↑
61	PIP(18:3(10,12,15)-OH(9)/16:0)	3.86	C43H78O17P2	929.480 5	1.93	[M+H]+	HMDB02785 04	↑**	↑
62	PIP(20:1(11Z)/18:1(12Z)-2OH(9,10))	5.96	C47H88O18P2	985.544 4	3.06	[M+H- H2O]+	HMDB02796 10	↑***	↑
63	PC(18:1(12Z)-O(9S,10R)/14:0)	17.18	C40H76NO9P	763.562 6	4.09	[M+NH4] +	HMDB02856 41	↑***	↑###
64	PC(LTE4/18:2(9Z,12Z))	7.75	C49H85N2O11 PS	958.596 0	1.09	[M+NH4] +	HMDB02865 53	↑**	↑
65	PC(20:5(5Z,8Z,11Z,14Z,16E)-OH(18R)/DiMe(9,5))	8.62	C48H80NO10P	884.547 3	7.03	[M+Na]+	HMDB02893 82	↑**	↑#
66	DG(PGF2alpha/10:0/0:0)	7.26	C33H58O8	1165.82 65	-6.08	[2M+H]+	HMDB02944 66	↓*	↓##
67	DG(20:5(6E,8Z,11Z,14Z,17Z)-OH(5)/10:0/0:0)	5.11	C33H54O6	1093.78 20	-8.61	[2M+H]+	HMDB02945 38	↑**	↑
68	DG(20:5(5Z,8Z,10E,14Z,17Z)-OH(12)/0:0/16:0)	4.49	C39H66O6	648.523 7	6.20	[M+NH4] +	HMDB02955 30	↑***	↓
69	DG(PGE2/17:0/0:0)	7.30	C40H70O8	1375.05 87	7.93	[2M+NH4] +]	HMDB02956 56	↓*	↓#
70	DG(TXB2/0:0/2:0)	7.82	C25H42O9	973.569 1	-4.02	[2M+H]+	HMDB02969 34	↑**	↑
71	(2E)-hept-2-enediyl-CoA	3.86	C28H44N7O19 P3S	930.148 8	-3.27	[M+Na]+	HMDB03014 46	↑***	↑
72	nona-4,6-dienoyl-CoA	7.83	C30H48N7O17 P3S	868.193 7	3.87	[M+H- 2H2O]+	HMDB03015 09	↑**	↑
73	22-Hydroxydocosanoic acid	7.43	C22H44O3	374.364 9	5.62	[M+NH4] +	HMDB03029 63	↑***	↑
74	4-hydroxysphinganine	5.87	C18H39NO3	318.303 3	9.42	[M+H]+	HMDB03041 83	↑*	↑

* P < 0.05, ** P < 0.01, *** P < 0.001, the Control group versus the Model group;

P < 0.05, ## P < 0.01, ### P < 0.001, the ZSD-H treatment group versus the Model group.