

Table S1 A Gradient elution program on T3 column.

Time (min)	Flow (mL/min)	A%	B%	Curve
0	0.2	100	0	—
0.5	0.2	100	0	6
20	0.2	5	95	6
21	0.2	5	95	6
24	0.2	100	0	1

B Gradient elution program on C18 column.

Time (min)	Flow (mL/min)	A%	B%	Curve
0	0.2	65	35	—
0.5	0.2	65	35	6
20	0.2	0	100	6
21	0.2	0	100	6
24	0.2	65	35	1

Table S2 Identification results of 14 potential biomarkers in lung tissue.

No.	<i>m/z</i>	Quasi-molecular ion	MS/MS		Fomula	Identification	CAS
1	103.9	[M + H] ⁺	60.0	45.0	C ₅ H ₁₃ NO	Choline	62-49-7
2	112.9	[M + H] ⁺	95.9	70.0	C ₄ H ₄ N ₂ O ₂	Uracil	66-22-8
3	118.0	[M + H] ⁺	58.8	57.1	C ₅ HNO ₂	Betaine	590-46-5
4	122.9	[M + H] ⁺	79.9	78.0	C ₆ H ₆ N ₂ O	Niacinamide	98-92-0
5	132.0	[M + H] ⁺	99.0	87.0	C ₄ H ₉ N ₃ O ₂	Creatine	57-00-1
6	136.9	[M + H] ⁺	118.8	109.8	C ₅ H ₄ N ₄ O	Hypoxanthine	68-94-0
			93.7	81.6			
7	153.0	[M + H] ⁺	136.0	110.0	C ₅ H ₄ N ₄ O ₂	Xanthine	69-89-6
8	162.1	[M + H] ⁺	103.0	60.1	C ₇ H ₁₅ NO ₃	Carnitine	541-15-1
9	274.3	[M + H] ⁺	256.3	239.2	C ₁₆ H ₃₅ NO ₂	C16 sphinganine	---
10	302.3	[M + H] ⁺	284.3	60.0	C ₁₈ H ₃₉ NO ₂	Sphinganine	764-22-7
11	318.3	[M + H] ⁺	300.3	256.3	C ₁₈ H ₃₉ NO ₃	Phytosphingosine	---
12	496.2	[M + H] ⁺	478.3	184.3	C ₂₄ H ₅₀ NO ₇ P	LPC (16:0)	---
			103.8	85.5			
13	524.3	[M + H] ⁺	506.4	184.0	C ₂₆ H ₅₄ NO ₇ P	LPC (18:0)	---
			103.8				
14	544.3	[M + H] ⁺	526.3	287.2	C ₂₈ H ₅₀ NO ₇ P	LPC (20:4)	---
			240.1				