Table S1: The information of biomarkers in the serum of lung cancer

NO	Rt/min	M/Z	Scan mode	M+X	Proposed composition	Predicting compound	HMDB ID	Mass Error (ppm)	Chang trend
1	2.55	514.2835	ESI+	M+H	$C_{26}H_{43}NO_7S$	Sulfolithocholylglycine	HMDB0002639	0.35	↓**
2	3.03	512.2683	ESI-	M-H	$C_{26}H_{43}NO_7S$	Sulfolithocholylglycine	HMDB0002639	-0.94	↓**
3	3.08	373.2741	ESI+	M+H	$C_{24}H_{36}O_3$	Cervonoyl ethanolamide	HMDB0013627	0.89	↑*
4	3.14	389.2688	ESI+	M+H	$C_{24}H_{36}O_4$	Cavipetin C	HMDB0030366	0.39	↑*
5	3.64	209.084	ESI-	M-H	$C_{11}H_{14}O_4$	Sinapyl alcohol	HMDB0013070	9.77	↑**
6	3.94	514.2833	ESI-	M-H	$C_{26}H_{45}NO_7S$	Taurocholic acid	HMDB0000036	-2.14	↓*
7	4.44	357.2794	ESI+	M+H	$C_{24}H_{36}O_2$	Tetracosahexaenoic acid	HMDB0002007	1.65	↑**
8	4.5	405.2638	ESI-	M-H	$C_{24}H_{38}O_5$	7-Ketodeoxycholic acid	HMDB0000391	-1.98	↑**
9	4.92	520.3403	ESI+	M+H	$C_{26}H_50NO_7P$	LysoPC(18:2(9Z,12Z))	HMDB0010386	1.03	↑**
10	4.93	544.34	ESI+	M+H	$C_{28}H_{50}NO_7P$	LysoPC(20:4(5Z,8Z,11Z,14Z))	HMDB0010395	0.42	↑**
11	5.02	498.2873	ESI-	M-H	$C_{26}H_{45}NO_6S$	Tauroursodeoxycholic acid	HMDB0000874	-4.43	↑**
12	5.13	544.3403	ESI+	M+H	$C_{28}H_{50}NO_7P$	LysoPC(20:4(5Z,8Z,11Z,14Z))	HMDB0010395	0.93	↑**
13	5.62	391.2844	ESI-	M-H	$C_{24}H_40O_4$	Allodeoxycholic acid	HMDB0000478	-2.56	↓**
14	5.7	496.34	ESI+	M+H	$C_{24}H_50NO_7P$	LysoPC(16:0)	HMDB0010382	0.43	↑**
15	5.7	518.3215	ESI+	M+H	$C_{26}H_{48}NO_7P$	LysoPC(18:3(6Z,9Z,12Z))	HMDB0010387	-4.99	↑**
16	5.76	522.3558	ESI+	M+H	$C_{26}H_{52}NO_7P$	LysoPC(18:1(9Z))	HMDB0002815	0.77	↑*
17	7.14	265.147	ESI-	M-H	$C_{15}H_{22}O_4$	Humulinic acid A	HMDB0030104	9.39	↑**
18	7.15	524.3714	ESI+	M+H	$C_{26}H_{54}NO_7P$	LysoPC(18:0)	HMDB0010384	0.65	↑**
19	7.15	546.3528	ESI+	M+H	$C_{28}H_{52}NO_7P$	LysoPC(20:3(5Z,8Z,11Z))	HMDB0010393	-4.72	↑**
20	7.96	256.2637	ESI+	M+H	$C_{16}H_{33}NO$	Palmitic amide	HMDB0012273	0.97	↓**
21	8.26	282.2795	ESI+	M+H	$C_{18}H_{35}NO$	Oleamide	HMDB0002117	1.33	↓**
22	8.5	480.3088	ESI-	M-H	$C_{23}H_{48}NO_7P$	LysoPC(15:0)	HMDB0010381	-1.49	↓*
23	8.75	112.9845	ESI-	M-H	$C_2HF_3O_2$	Trifluoroacetic acid	HMDB0014118	-9.9	↑**
24	9.3	782.5682	ESI+	M+H	$C_{44}H_80NO_8P$	PC(16:1(9Z)/20:3(5Z,8Z,11Z))	HMDB0008013	-1.59	↑**
25	9.31	758.572	ESI+	M+H	$C_{42}H_80NO_8P$	PC(14:0/20:2(11Z,14Z))	HMDB0007880	3.40	↑**
26	10.16	313.0776	ESI-	M-H	$C_{15}H_{14}N_4O_2S$	Sulfaphenazole	HMDB0015667	3.75	↑**
27	10.18	165.0398	ESI-	M-H	$C_5H_10O_6$	Arabinonic acid	HMDB0000539	-4.14	↑**
28	10.6	491.3381	ESI-	M-H	$C_{29}H_{48}O_6$	Homodolicholide	HMDB0033907	0.67	↓**
29	10.62	473.2896	ESI-	M-H	$C_{28}H_{42}O_6$	Pubescenol	HMDB0030085	-2.64	↑**
30	10.84	465.3061	ESI-	M-H	$C_{27}H_{46}O_4S$	Cholesterol sulfate	HMDB0000653	3.52	↑**
31	11.09	313.0777	ESI-	M-H	$C_{15}H_{14}N_4O_2S$	Sulfaphenazole	HMDB0015667	3.78	↑**

↑ It indicates that the metabolite content in the serum of the lung cancer model group is significantly higher than that of the control group;
↓It indicates that the metabolite content in the serum of the lung cancer model group is significantly lower than that of the control group;

Table S2: Trends of potential biomarker treatment with high dose of chuanxiong group, low dose of chuanxiong group and protamine group.

NO	Rt/min	M/Z	Predicting compound	Chang trend	HD	LD	PTM
1	2.55	514.2835	Sulfolithocholylglycine	↓**	+##	+#	+
2	3.03	512.2683	Sulfolithocholylglycine	↓**	+##	+#	+##
3	3.08	373.2741	Cervonoyl ethanolamide	↑*	+##	+##	+##
4	3.14	389.2688	Cavipetin C	↑*	+#	+##	+#
5	3.64	209.084	Sinapyl alcohol	↑**	+##	-	-
6	3.94	514.2833	Taurocholic acid	↓*	-	+#	+##
7	4.44	357.2794	Tetracosahexaenoic acid	↑**	+##	+##	+##
8	4.5	405.2638	7-Ketodeoxycholic acid	↑**	+	+	+##
9	4.92	520.3403	LysoPC(18:2(9Z,12Z))	↑**	+##	+##	+##
10	4.93	544.34	LysoPC(20:4(5Z,8Z,11Z,14Z))	↑**	+##	+##	+##
11	5.02	498.2873	Tauroursodeoxycholic acid	↑**	-	+#	+##
12	5.13	544.3403	LysoPC(20:4(5Z,8Z,11Z,14Z))	↑**	+##	+##	+##
13	5.62	391.2844	Allodeoxycholic acid	↓**	+	+#	+##
14	5.7	496.34	LysoPC(16:0)	↑**	+##	+##	+##
15	5.7	518.3215	LysoPC(18:3(6Z,9Z,12Z))	↑**	+##	+##	+##
16	5.76	522.3558	LysoPC(18:1(9Z))	↑*	+##	+##	+##
17	7.14	265.147	Humulinic acid A	↑**	+##	+	+
18	7.15	524.3714	LysoPC(18:0)	↑**	+##	+##	+##
19	7.15	546.3528	LysoPC(20:3(5Z,8Z,11Z))	↑**	+##	+##	+##
20	7.96	256.2637	Palmitic amide	↓**	+##	+##	+##
21	8.26	282.2795	Oleamide	↓**	+##	+##	+##
22	8.5	480.3088	LysoPC(15:0)	↓*	+	-	-
23	8.75	112.9845	Trifluoroacetic acid	↑**	+##	+##	+##
24	9.3	782.5682	PC(16:1(9Z)/20:3(5Z,8Z,11Z))	↑**	+##	+##	+##
25	9.31	758.572	PC(14:0/20:2(11Z,14Z))	↑**	+##	+##	+##
26	10.16	313.0776	Sulfaphenazole	↑**	-	+	+
27	10.18	165.0398	Arabinonic acid	↑**	+	+	+
28	10.6	491.3381	Homodolicholide	↓**	+	-	-
29	10.62	473.2896	Pubescenol	↑**	+#	-	-
30	10.84	465.3061	Cholesterol sulfate	↑**	+#	-	+
31	11.09	313.0777	Sulfaphenazole	↑**	+#	-	-

↑ It indicates that the metabolite content in the serum of the lung cancer model group is significantly higher than that of the control group;
↓It indicates that the metabolite content in the serum of the lung cancer model group is significantly lower than that of the control group;
+ Callback trend **c**ompared with the model group;
- There is no callback trend compared to the model group:
(*P<0.05;**P<0.01.# P<0.05； ## P<0.01)

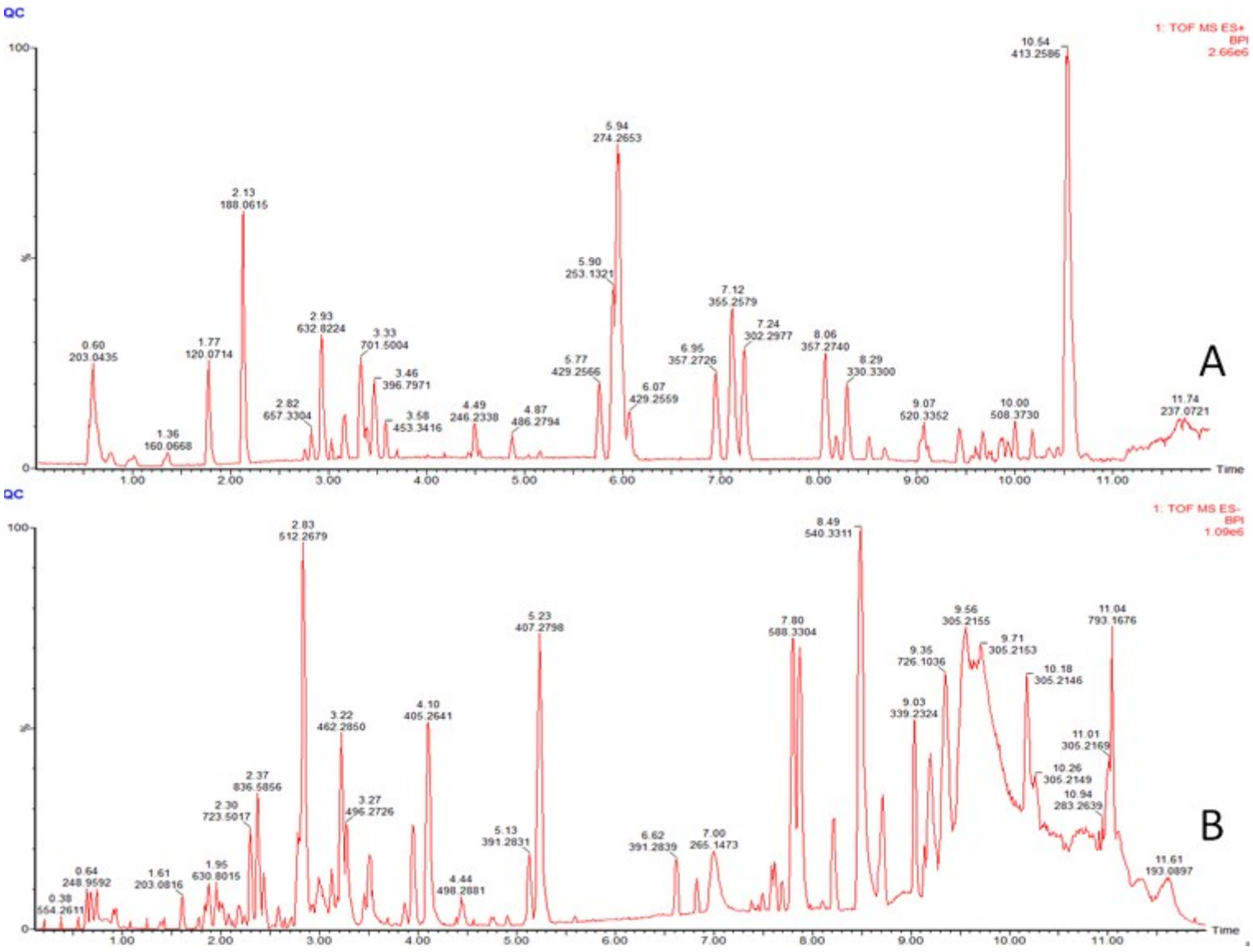

Fig.S1. UPLC-MS BPI ion map of QC. (A) Positive ion mode. (B) Negative ion mode.

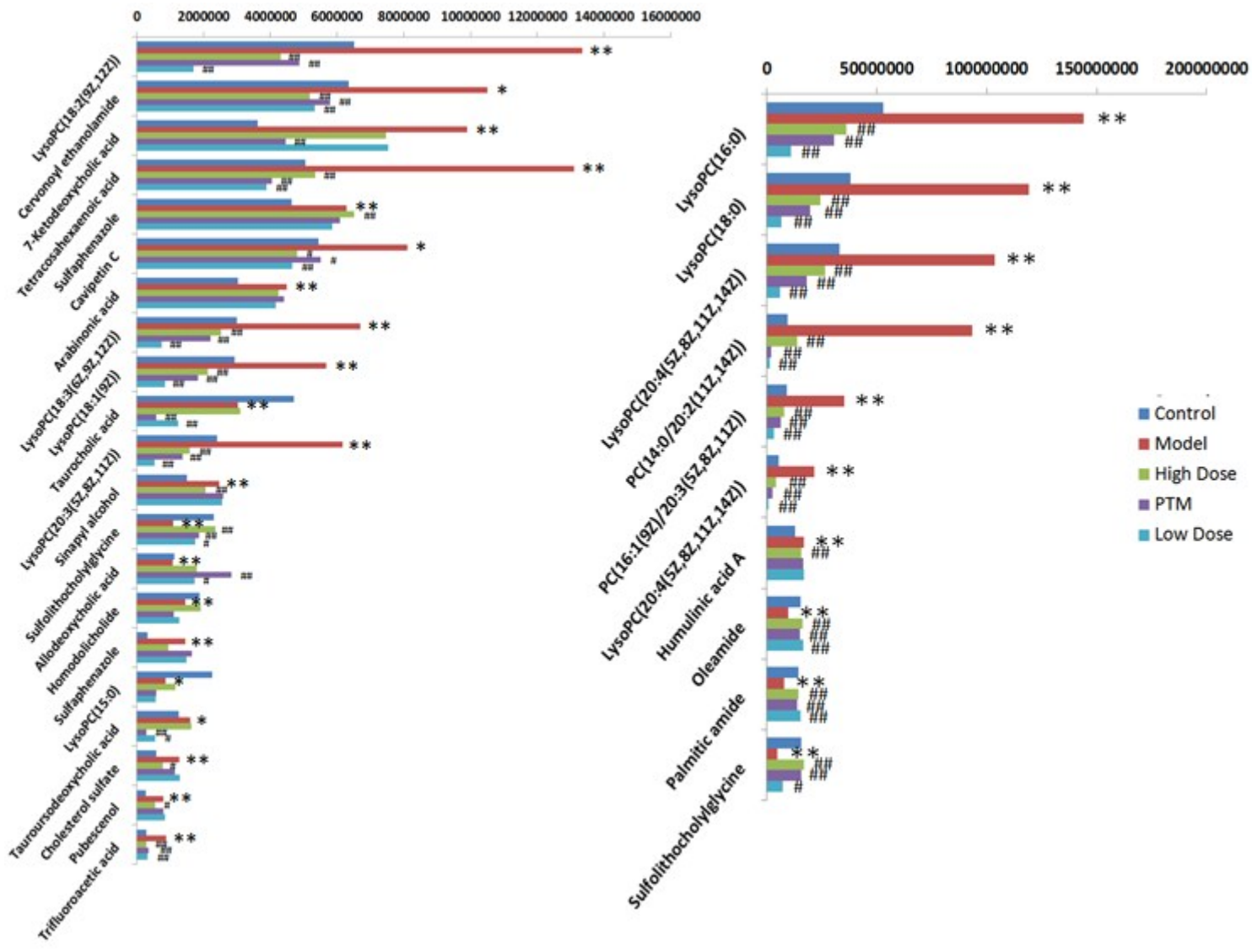

Fig.S2.The relative content of 31 potential biomarkers in each group of mice after treatment with CX solution was given. (Compare the control group to the model group, *P<0.05, **P<0.01; comparison between model group and other group, # P<0.05，##P<0.01. ）