Electronic Supplementary Information for

Comparative Study of Alterations in Phospholipid Profiles upon Liver Cancer in Humans and Mice

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Serum Preparation

Blood samples were collected after overnight fasting of the subjects. The collected blood samples were centrifuged at 3000 rpm for 10 min at 4 ℃ (Allegra 64R Centrifuge, Beckman Coulter) for obtaining serum samples. For DI-ESI-MS analysis, serum sample preparation referred to the earlier literature.[1] As a first step, 100μl of thawed serum sample under 4 ℃ was added into a labeled 1.5 ml Eppendorf vial. Next, protein precipitation and phospholipids extraction were performed by adding 300 μl methanol, the mixture was vortexed for 15 s and stored at -20 ℃ for 20 min. Then, each sample was centrifuged at 12000 rpm for 10 min at 4 ℃, and 200 μl supernatant was collected into labeled 1.5 ml Eppendorf vial for DI-ESI-MS analysis.

Analysis of Serum by DI-ESI-MS

For DI-ESI-MS analysis, all samples were diluted 200 times using methanol to avoid the contaminants to instrument. The DI-ESI-MS experiments were carried out using an Orbitrap Fusion Tribrid mass spectrometer (Thermo Scientific, San Jose, CA, United States). Mass spectra were collected in the mass range of *m/z* 400-1100. The positive ESI-MS spray voltage was 3.5 kV. The sheath gas pressure was 20 instrument units. The ion transfer tube temperature and vaporizer temperature were kept at 320 ℃ and 25 ℃, respectively. Each sample was analyzed in eight replicates.

1. D. Wang, S. L. Cheng, Q. Fei, H. Gu, D. Raftery, B. Cao, X. Sun, J. Yan, C. Zhang and J. Wang, *Psychiat. Res.*, 2019, **272**, 18-29.

Table S1. Chemical assignment for signals from tissue and serum samples.

No.	Compounds	Molecular formula	*Accurate m/z*	*Theoretical m/z*	Error(ppm)	Ion formation	MS/MS fragments
1	SM(34:1)	$C_{39}H_{79}N_2O_6P$	725.5586	725.5568	2	$[M + Na]^+$	666/542
2	SM(34:1)	$C_{39}H_{79}N_2O_6P$	741.5287	741.5307	3	$[M + K]^+$	682/558
3	PC(32:0)	$C_{40}H_{80}NO_8P$	756.5535	756.5514	3	$[M + Na]^+$	698/574
4	PC(32:0)	$C_{40}H_{80}NO_8P$	772.5231	772.5253	3	$[M + K]^+$	714
5	PC(34:2)	$C_{42}H_{80}NO_8P$	758.5710	758.5694	2	$[M + H]^+$	699/575
6	PC(34:2)	$C_{42}H_{80}NO_8P$	780.5545	780.5514	4	$[M + Na]^+$	721/597
7	PC(34:2)	$C_{42}H_{80}NO_8P$	796.5268	796.5253	2	$[M + K]^+$	737/614
8	PC(36:4)	$C_{44}H_{81}NO_8P$	782.5711	782.5694	2	$[M + H]^+$	723/599
9	PC(36:4)	$C_{44}H_{81}NO_8P$	804.5534	804.5538	0	$[M + Na]^+$	745/621
10	PC(36:4)	$C_{44}H_{81}NO_8P$	820.5225	820.5253	3	$[M + K]^+$	761/637
11	PC(34:1)	$C_{42}H_{82}NO_8P$	798.5387	798.5410	3	$[M + K]^+$	740/616
12	PC(36:2)	$C_{44}H_{84}NO_8P$	786.6038	786.6007	4	$[M + H]^+$	727/645
13	PC(36:2)	$C_{44}H_{84}NO_8P$	808.5802	808.5827	3	$[M + Na]^+$	750/626
14	PC(36:2)	$C_{44}H_{84}NO_8P$	824.5540	824.5566	3	$[M + K]^+$	766/642
15	PC(38:4)	$C_{46}H_{84}NO_8P$	810.6018	810.6007	1	$[M + H]^+$	752/628
16	PC(38:4)	$C_{46}H_{84}NO_8P$	832.5799	832.5827	3	$[M + Na]^+$	774/650
17	PC(38:4)	$C_{46}H_{84}NO_8P$	848.5539	848.5566	3	$[M + K]^+$	790/666
18	PA(37:6)	$C_{40}H_{67}NO_8P$	745.4206	745.4205	0	$[M + K]^+$	713/621
19	PC(40:9)	$C_{48}H_{78}NO_8P$	828.5534	828.5538	0	$[M + H]^+$	769/645
20	PC(38:6)	$C_{46}H_{80}NO_8P$	806.5689	806.5694	1	$[M + H]^+$	747/624
21	PC(42:9)	$C_{50}H_{82}NO_8P$	856.5853	856.5851	1	$[M + H]^+$	798/674

Table S2. The list of signals (VIP > 1.0) that made major contributions to differentiate different sample groups.

Human tissue				Mouse tissue				Human serum			
m/z	**VIP value**	***m/z***	**VIP value**	***m/z***	**VIP value**	***m/z***	**VIP value**	***m/z***	**VIP value**	***m/z***	**VIP value**
733	2.3794	833	1.28675	773	3.62778	851	1.30406	805	2.76751	775	1.3645
759	1.88311	807	1.28437	845	3.07593	801	1.28012	833	2.65499	810	1.35514
823	1.86643	897	1.28202	774	2.60883	810	1.23421	807	2.50083	816	1.35162
882	1.85497	877	1.27225	846	2.44295	807	1.23168	814	2.42166	733	1.34682
771	1.82263	741	1.26714	799	2.42491	787	1.21953	784	2.33634	785	1.34589
757	1.82185	878	1.2607	771	2.40165	833	1.20467	783	2.31688	734	1.3274
872	1.80231	805	1.23961	825	2.27269	781	1.19405	831	2.24655	709	1.32051
797	1.7968	900	1.23837	797	2.11489	742	1.19044	809	2.22894	722	1.2977
761	1.72105	826	1.23707	827	1.99163	829	1.18259	747	2.13921	882	1.23076
726	1.69883	735	1.22889	826	1.91464	783	1.17435	710	2.09982	859	1.19399
755	1.68951	799	1.21653	798	1.88638	811	1.16821	806	2.06853	822	1.19244
783	1.66545	796	1.20925	873	1.8632	808	1.11181	821	2.03602	712	1.18668
870	1.58203	819	1.19828	772	1.83337	782	1.10282	858	1.96763	857	1.17567
851	1.5727	817	1.17656	800	1.81875	735	1.08574	829	1.93484	708	1.17186
779	1.52028	881	1.16252	849	1.78788	760	1.04007	720	1.82965	750	1.16124
821	1.51691	834	1.16246	757	1.6345	857	1.03353	808	1.82368	726	1.08095
787	1.45016	760	1.16177	775	1.62493	746	1.029	759	1.79345	872	1.07786
849	1.44399	717	1.13954	823	1.60569	830	1.0212	834	1.76201	870	1.07453
781	1.4379	800	1.13728	847	1.56536	812	1.01108	776	1.63569	815	1.05913
856	1.43284	844	1.1153	822	1.51394			835	1.57841	855	1.01747
845	1.42794	852	1.11432	758	1.47691			778	1.57558	794	1.01003
795	1.42525	850	1.09766	874	1.46825			854	1.56323	767	1.01001
739	1.40891	859	1.08669	809	1.44878			844	1.46395		
769	1.40422	811	1.08529	819	1.42884			898	1.44547		
825	1.39791	767	1.06322	745	1.42782			866	1.42449		
740	1.38374	824	1.03907	821	1.3873			706	1.41925		
898	1.36148	831	1.03858	784	1.36864			766	1.40665		
884	1.35164	773	1.03223	850	1.35245			832	1.38359		
791	1.34623	734	1.02822	759	1.34902			895	1.38322		
857	1.32709	883	1.02458	824	1.33866			830	1.37124		
809	1.31355	756	1.01069	828	1.32343			838	1.3666		

Table S3. The list of the importance of signal features that are used to predict liver cancer in the random forest model.

m/z	significance	*m/z*	significance	*m/z*	significance	*m/z*	significance	*m/z*	significance
701	0.069768	741	0.286483	781	0.535175	821	0.230881	861	0.339997
702	0.591454	742	0.734353	782	0.367831	822	0.83992	862	0.211984
703	0.390325	743	1.299298	783	0.098858	823	1.763338	863	0.292297
704	1.149526	744	0.290318	784	0.130899	824	0.142469	864	0.177599
705	0.274289	745	0.553727	785	0.149389	825	0.370823	865	0.186992
706	2.638271	746	0.45099	786	0.315065	826	0.198789	866	2.078227
707	0.87653	747	0.408593	787	0.616762	827	0.242734	867	0.305469
708	0.785582	748	0.300302	788	0.5173	828	0.360736	868	0.20348
709	1.136774	749	0.32201	789	0.21924	829	0.321271	869	0.408671
710	0.548553	750	0.225379	790	0.076467	830	0.314364	870	2.146491
711	0.148665	751	0.240252	791	0.97885	831	0.228203	871	0.091805
712	0.511026	752	0.828356	792	0.753034	832	0.128711	872	0.323609
713	0.313514	753	0.279998	793	0.271983	833	0.177641	873	0.359209
714	0.1398	754	0.429618	794	0.276039	834	0.161003	874	0.190444
715	1.288191	755	0.288254	795	0.179643	835	0.247803	875	0.797682
716	0.141756	756	0.373611	796	0.21431	836	0.104223	876	0.35806
717	0.399322	757	0.242928	797	0.19931	837	0.59676	877	1.467637
718	0.211278	758	0.30848	798	0.228373	838	3.523515	878	0.33007
719	0.546985	759	0.485696	799	0.139049	839	0.203709	879	0.346099
720	0.789761	760	0.364871	800	0.739107	840	0.241764	880	0.825889
721	0.258434	761	0.233425	801	0.075952	841	0.369065	881	0.142615
722	2.105688	762	0.101748	802	0.466305	842	0.232641	882	1.879974
723	0.467576	763	1.414282	803	0.492929	843	0.261604	883	0.174729
724	0.611476	764	0.531795	804	0.296047	844	0.333512	884	0.294112
725	0.407433	765	0.97183	805	0.187451	845	0.760019	885	0.300167
726	0.458377	766	1.172727	806	0.224058	846	0.266788	886	0.447865
727	0.316076	767	0.153124	807	0.234171	847	0.200385	887	0.270292
728	0.34082	768	0.342868	808	0.26369	848	0.128724	888	0.394723
729	0.397322	769	0.241416	809	0.303223	849	0.33597	889	0.878944
730	0.144291	770	0.249807	810	0.204429	850	0.645138	890	0.212534
731	0.558819	771	0.121651	811	0.182058	851	1.07167	891	0.949184
732	0.549667	772	0.130608	812	0.1879	852	0.248842	892	0.202053
733	0.973644	773	0.439734	813	0.23259	853	0.111629	893	3.542242
734	6.518674	774	0.100179	814	0.611412	854	1.635022	894	1.22372
735	0.74386	775	0.696211	815	0.233168	855	0.335419	895	0.218404
736	0.170876	776	0.777451	816	0.267671	856	0.090813	896	0.551663
737	0.25067	777	0.684957	817	0.221142	857	0.612513	897	0.239048
738	0.143737	778	4.606335	818	0.224839	858	0.297996	898	4.652004
739	0.172284	779	0.173005	819	0.213009	859	0.234755	899	0.140153
740	0.229381	780	0.203082	820	0.080842	860	0.389737	900	0.396969