Electronic Supplementary Information for：

Internal extractive electrospray ionization mass spectrometry for the phospholipid-dysregulation investigation of perfluorooctanoic acid on Nile tilapia

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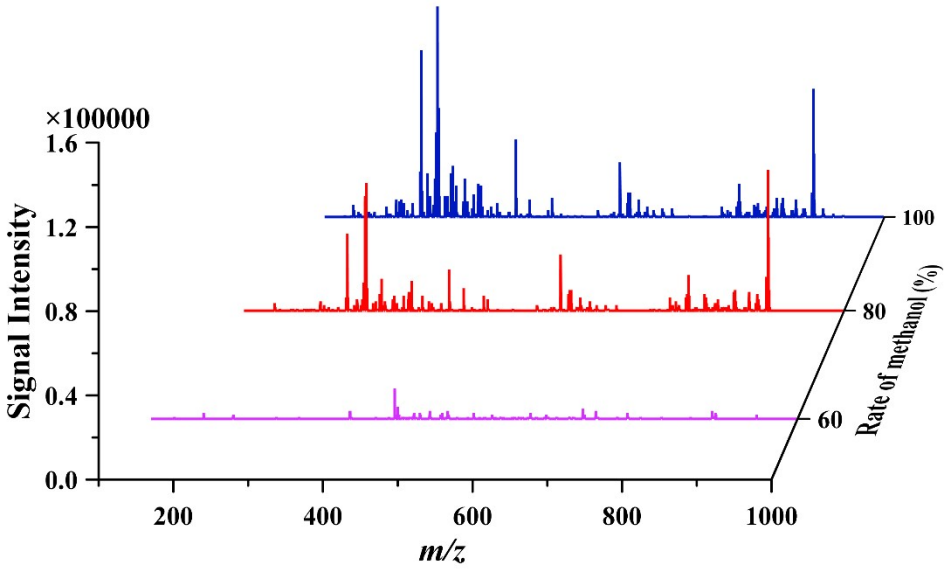

Fig. S1 Mass spectra of a liver sample detected by iEESI-MS in negative ion detection mode with 3 extraction solutions.

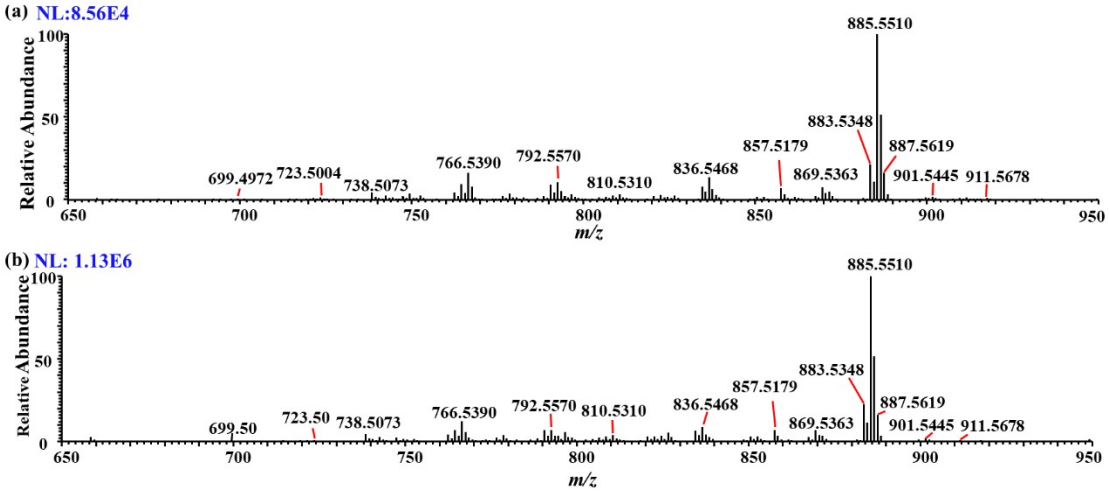

Fig. S2 Mass spectra of a liver sample detected by iEESI-MS in negative ion detection mode with 2 extraction solutions. (a) CH_3OH/H_2O (80:20, v/v) and (b) $CH_3OH/H_2O/NH_4OH$ (80:20:0.3, v/v/w).

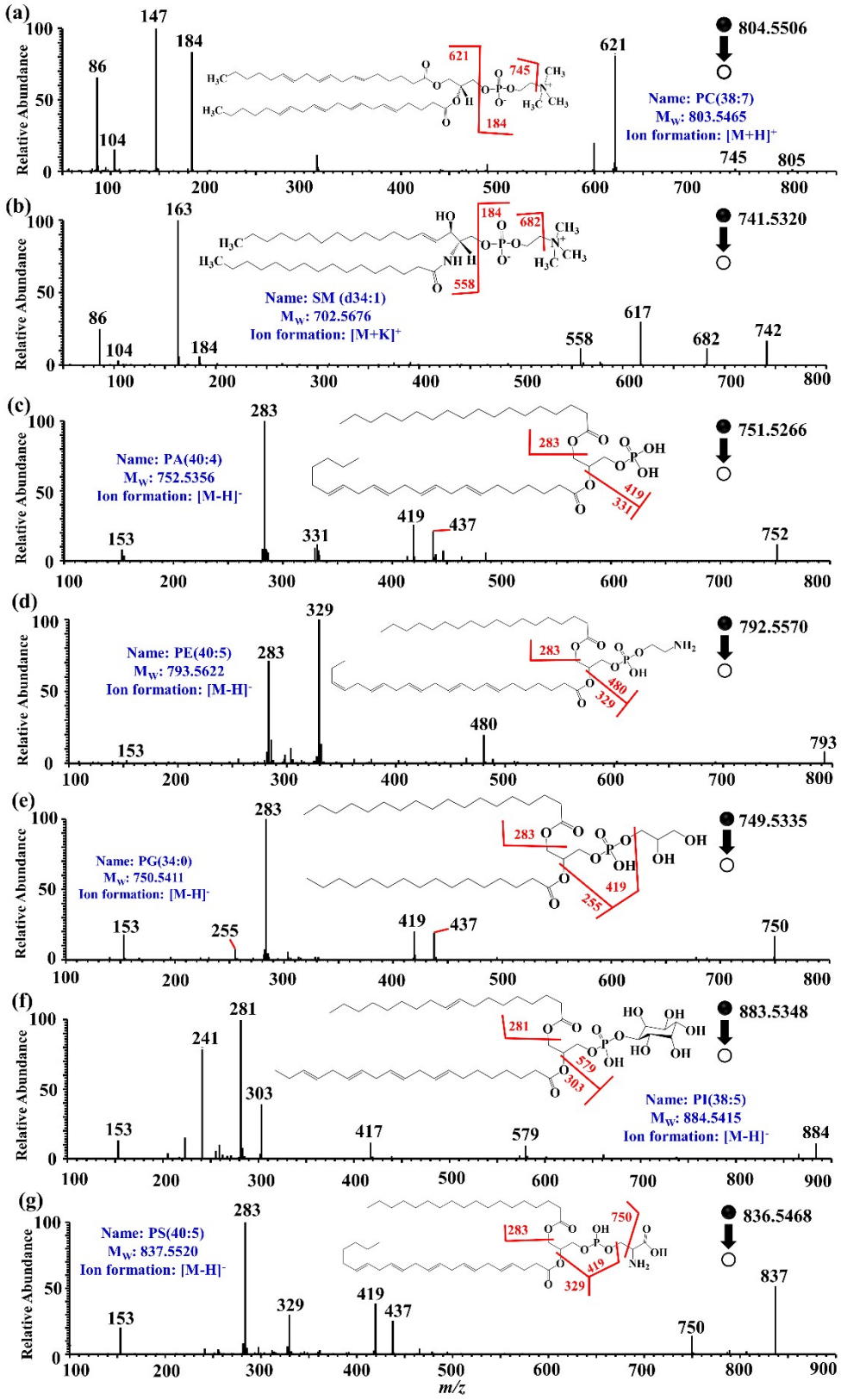

Fig. S3 Identification of representative phospholipid species. (a) PC (38:7), (b) SM (d34:1), (c) PA (40:4), (d) PE (40:5), (e) PG (34:0), (f) PI (38:5) and (g) PS (40:5).

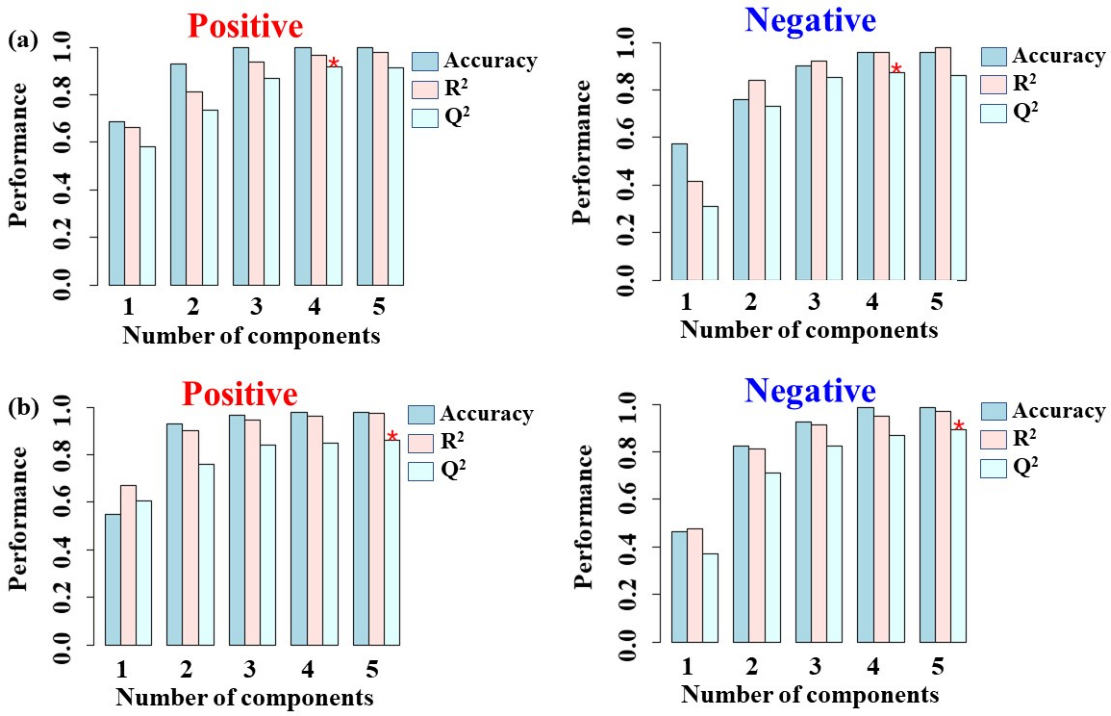

Fig. S4 CV score of PLS-DA models in different tissue samples. (a) liver sample, (b) spleen sample. Q^2, R^2 and Accuracy values are three common performance measures of PLS-DA model. And the default criterion is Q^2 value, which indicates the predictive ability of the PLS-DA model (red asterisk denotes optimal Q^2 value).

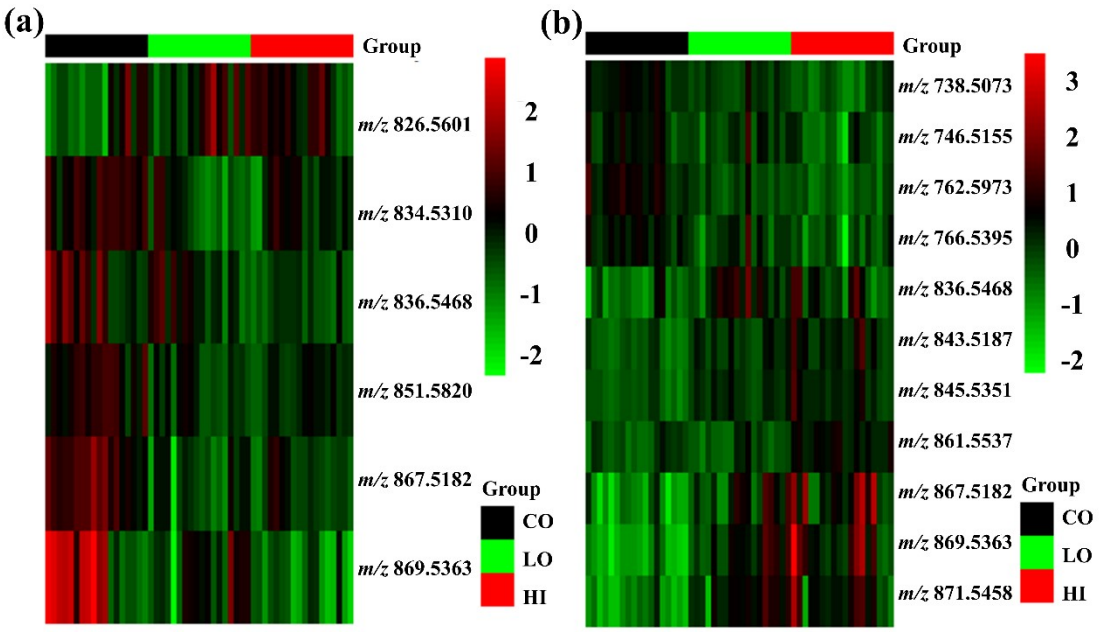

Fig. S5 Heatmap of dysregulated phospholipid signals detected by iEESI-MS in negative ion detection mode in tissue samples of Nile tilapia exposed to PFOA. (a) liver sample, (b) spleen sample.

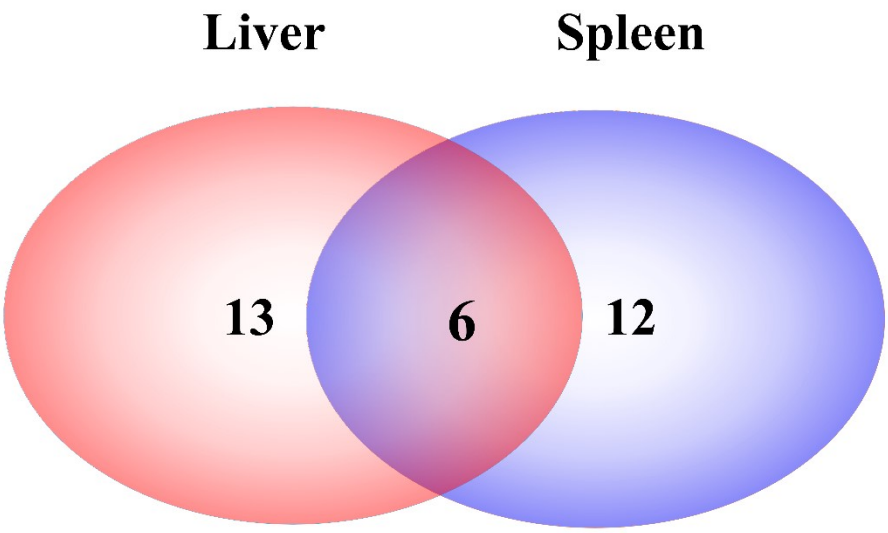

Fig. S6: Venn diagram displays the coverage of differential phospholipid signals in liver and spleen samples of Nile tilapia.

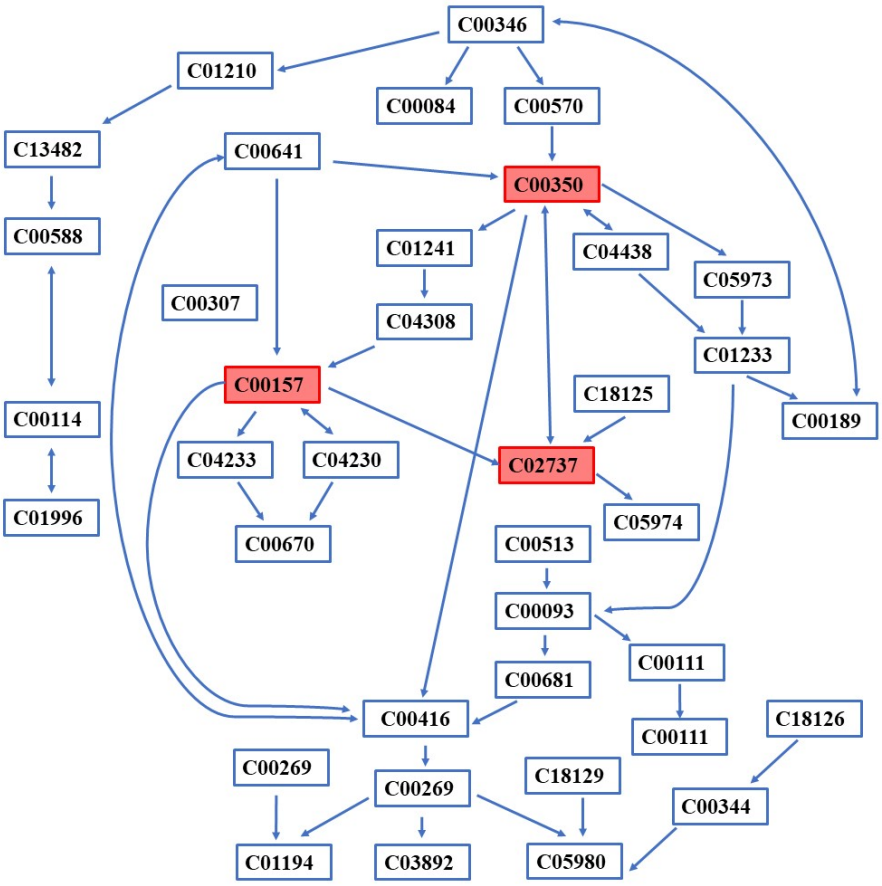

Fig. S7 Graphical presentation of the glycerophospholipid metabolism and involved dysregulated phospholipid species (marked in red) in this study. (C00157, C00350 and C02737 respectively refer to PC, PE and PS).

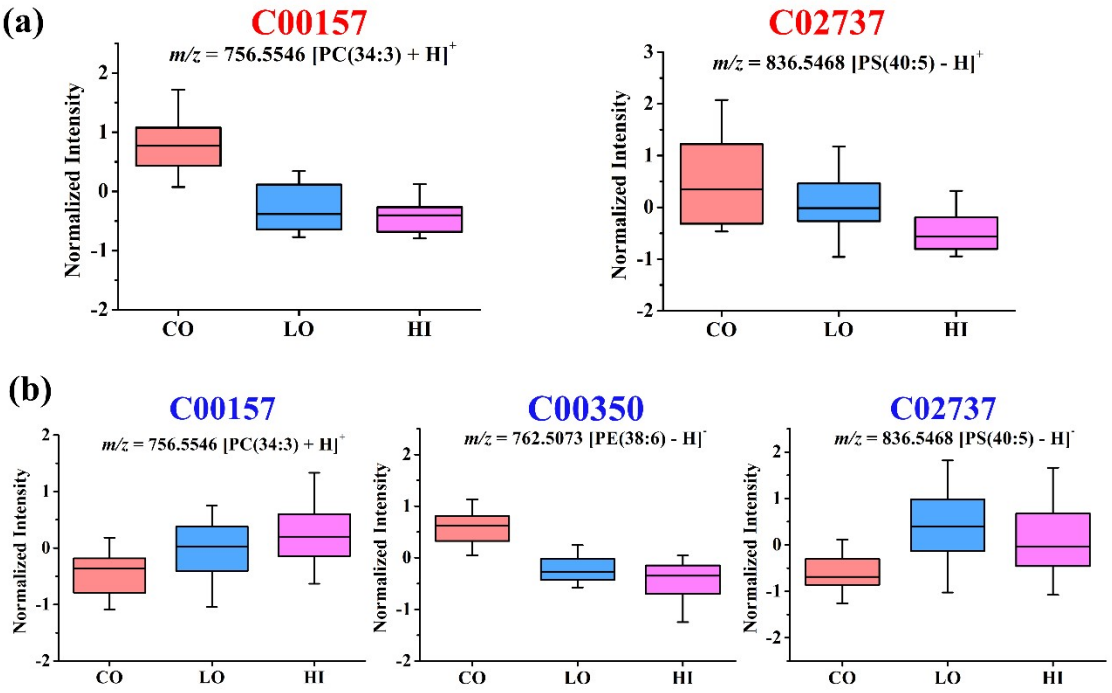

Fig. S8 Boxplot analysis of disturbed phospholipid signals in glycerophospholipid metabolism pathway in the liver (a) and spleen(b). In liver and spleen, 2 (PCs, PSs) and 3 (PCs, PSs, PEs) differential phospholipid species were separately involved in glycerophospholipid metabolism pathway, and one phospholipid signal is selected from each category of phospholipid species as representative for boxplot analysis. (C00157, C00350 and C02737 respectively refer to PC, PE and PS).

Table S1 Identification of phospholipid sginals detected by iEESI-MS in the positive and negative ion detection mode.

NO	Compound name	Experimental *m/z*	Theoretical *m/z*	Formula	Ion Formation	MS/MS Fragments	Error (ppm)	Model
1	SM (d34:4)	697.5260	697.5279	$C_{39}H_{73}N_2O_6P$	$[M+H]^+$	104/147/184/514/638	3	Positive
2	SM (d34:1)	703.5755	703.5748	$C_{39}H_{79}N_2O_6P$	$[M+H]^+$	104/125/184/644/520	1	Positive
3	SM (d34:1)	741.5320	741.5307	$C_{39}H_{79}N_2O_6P$	$[M+K]^+$	163/184/682/558	2	Positive
4	SM (d32:1)	713.5002	713.4994	$C_{37}H_{75}N_2O_6P$	$[M+K]^+$	163/184/530/654	1	Positive
5	SM (d36:4)	725.5564	725.5592	$C_{41}H_{77}N_2O_6P$	$[M+H]^+$	104/147/184/542/666	3	Positive
6	PC (32:2)	730.5382	730.5381	$C_{40}H_{76}NO_8$	$[M+H]^+$	86/104/184/671	0	Positive
7	PC (32:1)	732.5548	732.5538	$C_{40}H_{78}NO_8P$	$[M+H]^+$	125/184/549/673	1	Positive
8	PC (32:0)	734.5709	734.5694	$C_{40}H_{80}NO_8P$	$[M+H]^+$	104/125/184/675	2	Positive
9	PC (34:4)	754.5374	754.5381	$C_{42}H_{76}NO_8P$	$[M+H]^+$	86/104/184/571/695	1	Positive
10	PC (34:3)	756.5546	756.5538	$C_{42}H_{78}NO_8P$	$[M+H]^+$	86/104/184/573/697	1	Positive
11	PC (34:2)	758.5707	758.5694	$C_{42}H_{80}NO_8P$	[M+H]	86/104/184/575/699	2	Positive
12	PC (34:1)	760.5858	760.5851	$C_{42}H_{82}NO_8P$	$[M+H]^+$	86/104/184/701	1	Positive
13	PC (32:2)	768.4954	768.4940	C40H76NO8P	$[M+K]^+$	86/104/184/709	2	Positive
14	PC (32:1)	770.5111	770.5097	C40H78NO8P	$[M+K]^+$	86/104/147/163/184/587/711	1	Positive

15	PC (32:0)	772.5272	772.5253	C40H80NO8P	$[M+K]^+$	104/163/184/589/713	1	Positive
16	PC (36:6)	778.5371	778.5381	$C_{44}H_{76}NO_8P$	$[M+H]^+$	86/104/147/184/595/719	1	Positive
17	PC (36:5)	780.5528	780.5538	$C_{44}H_{78}NO_8P$	$[M+H]^+$	86/104/125/146/184/597/721	1	Positive
18	PC (36:4)	782.5688	782.5694	$C_{44}H_{80}NO_8P$	$[M+H]^+$	86/104/147/184/599/723	1	Positive
19	PC (36:3)	784.5859	784.5851	$C_{44}H_{82}NO_8P$	$[M+H]^+$	86/104/184/601/725	1	Positive
20	PC (36:2)	786.6019	786.6007	$C_{44}H_{84}NO_8P$	$[M+H]^+$	86/104/184/603/727	2	Positive
21	PC (34:4)	792.4957	792.4940	$C_{42}H_{76}NO_8P$	$[M+K]^+$	86/104/163/184/609/733	2	Positive
22	PC (34:3)	794.5110	794.5097	$C_{42}H_{78}NO_8P$	$[M+K]^+$	86/104/184/735	0	Positive
23	PC (34:2)	796.5269	796.5253	$C_{42}H_{80}NO_8P$	$[M+K]^+$	86/104/163/184/613/737	2	Positive
24	PC (34:1)	798.5389	798.5410	$C_{42}H_{82}NO_8P$	$[M+K]^+$	86/104/163/184/615/739	3	Positive
25	PC (38:8)	802.5354	802.5381	$C_{46}H_{80}NO_8P$	[M+H] +	86/104/147/184/619/743	3	Positive
26	PC (38:7)	804.5506	804.5538	$C_{46}H_{78}NO_8P$	$[M+H]^+$	86/104/147/184/621/745	4	Positive
27	PC (38:6)	806.5660	806.5694	$C_{46}H_{80}NO_8P$	$[M+H]^+$	86/104/147/184/747	4	Positive
28	PC (38:5)	808.5826	808.5851	$C_{46}H_{82}NO_8P$	$[M+H]^+$	86/104/147/184/625/749	3	Positive
29	PC (36:5)	818.5099	818.5097	$C_{44}H_{78}NO_8P$	$[M+K]^+$	86/104/163/184/635/759	0	Positive
30	PC (36:4)	820.5253	820.5253	$C_{44}H_{80}NO_8P$	$[M+K]^+$	86/104/184/637/761	0	Positive
31	PC (36:3)	822.5399	822.5410	$C_{44}H_{82}NO_8P$	$[M+K]^+$	86/104/184/639/763	2	Positive

32	PC (36:2)	824.5543	824.5566	$C_{44}H_{84}NO_8P$	$[M+K]^+$	86/104/184/641/765	3	Positive
33	PC (36:1)	826.5730	826.5723	$C_{44}H_{86}NO_8P$	$[M+K]^+$	86/104/163/184/643/767	1	Positive
34	PC (40:9)	828.5521	828.5538	$C_{48}H_{78}NO_8P$	$[M+H]^+$	86/104/147/184/645/769	2	Positive
35	PC (40:8)	830.5680	830.5694	$C_{48}H_{80}NO_8P$	$[M+H]^+$	86/104/147/184/647/771	2	Positive
36	PC (40:7)	832.5842	832.5851	$C_{48}H_{82}NO_8P$	$[M+H]^+$	86/104/184/649/773	1	Positive
37	PC (38:7)	842.5091	842.5097	$C_{46}H_{78}NO_8P$	$[M+K]^+$	86/104/163/184/659/783	1	Positive
38	PC (38:6)	844.5246	844.5253	$C_{46}H_{80}NO_8P$	$[M+K]^+$	86/104/163/184/661/785	1	Positive
39	PC (38:5)	846.5418	846.5410	$C_{46}H_{82}NO_8P$	$[M+K]^+$	104/163/184/787	1	Positive
40	PC (38:4)	848.5582	848.5566	$C_{46}H_{84}NO_8P$	$[M+K]^+$	86/104/163/184/665/789	2	Positive
41	PC (38:3)	850.5711	850.5723	$C_{46}H_{86}NO_8P$	$[M+K]^+$	86/104/163/184/667/791	1	Positive
42	PC (38:2)	852.5891	852.5879	$C_{46}H_{88}NO_8P$	$[M+K]^+$	86/104/184/669	1	Positive
43	PC (42:10)	854.5678	854.5694	$C_{50}H_{80}NO_8P$	$[M+H]^+$	86/104/147/184/671/795	2	Positive
44	PC (42:9)	856.5835	856.5851	$C_{52}H_{80}NO_8P$	$[M+H]^+$	86/104/147/184/673/797	2	Positive
45	PC (40:8)	868.5265	868.5253	$C_{48}H_{80}NO_8P$	$[M+K]^+$	86/104/163/184/685/809	1	Positive
46	PC (40:7)	870.5419	870.5410	$C_{48}H_{82}NO_8P$	$[M+K]^+$	86/104/163/184/687/811	1	Positive
47	PC (40:6)	872.5576	872.5566	$C_{48}H_{84}NO_8P$	$[M+K]^+$	86/104/184/813	1	Positive
48	PC (40:5)	874.5740	874.5723	$C_{48}H_{86}NO_8P$	$[M+K]^+$	86/104/163/184/691/815	2	Positive

49	PC (40:4)	876.5868	876.5879	$C_{48}H_{88}NO_8P$	$[M+K]^+$	86/104/163/184/693	1	Positive
50	PC (44:12)	916.5226	916.5253	$C_{52}H_{80}NO_8P$	$[M+K]^+$	86/104/163/184/733/857	3	Positive
51	PA (36:1)	701.515	701.5127	$C_{39}H_{75}O_8P$	$[M-H]^-$	281/283/417/419/437	3	Negative
52	PA (36:2)	699.4972	699.4970	$C_{39}H_{73}O_8P$	$[M-H]^-$	279/283/415/419/437	0	Negative
53	PA (38:3)	725.5129	725.5127	$C_{41}H_{75}O_8P$	$[M-H]^-$	283/305/419/437	0	Negative
54	PA (38:4)	723.5004	723.4970	$C_{41}H_{73}O_8P$	$[M-H]^-$	153/283/303/419/437	5	Negative
55	PA (38:5)	721.4830	721.4814	$C_{41}H_{71}O_8P$	$[M-H]^-$	153/255/329	2	Negative
56	PA (40:4)	751.5266	751.5283	$C_{43}H_{77}O_8P$	$[M-H]^-$	153/283/331/419/437	2	Negative
57	PA (40:5)	749.5111	749.5127	$C_{43}H_{75}O_8P$	$[M-H]^-$	153/283/329/419/437	2	Negative
58	PE (34:0)	718.5410	718.5392	$C_{39}H_{78}NO_8P$	$[M-H]^-$	255/283/462	0	Negative
59	PE (34:1)	716.5250	716.5236	$C_{39}H_{76}NO_8P$	$[M-H]^-$	153/255/281/460	2	Negative
60	PE (34:2)	714.508	714.5079	$C_{39}H_{74}NO_8P$	$[M-H]^-$	140/255/279/452	0	Negative
61	PE (34:3)	712.4912	712.4923	$C_{39}H_{72}NO_8P$	$[M-H]^-$	153/253/279	0	Negative
62	PE (36:1)	744.5570	744.5549	$C_{41}H_{80}NO_8P$	$[M-H]^-$	153/281/283	3	Negative
63	PE (36:2)	742.5415	742.5392	$C_{41}H_{78}NO_8P$	$[M-H]^-$	279/283/476/478	3	Negative
64	PE (36:3)	740.5262	740.5236	$C_{41}H_{76}NO_8P$	$[M-H]^-$	279/281/476	3	Negative
65	PE (36:4)	738.5073	738.5079	$C_{41}H_{74}NO_8P$	$[M-H]^-$	255/303/452	0	Negative

66	PE (38:3)	768.5527	768.5549	$C_{43}H_{80}NO_8P$	$[M-H]^-$	283/305/462/480	2	Negative
67	PE (38:4)	748.5290	748.5281	$C_{43}H_{78}NO_8P$	$[M-H_2O-H]^-$	140/153/283/303	1	Negative
68	PE (38:4)	766.5395	766.5392	$C_{43}H_{78}NO_8P$	$[M-H]^-$	140/153/283/303/480	1	Negative
69	PE (38:4; O)	782.5350	782.5342	$C_{43}H_{78}NO_9P$	$[M-H]^-$	153/303/448/466	1	Negative
70	PE (38:5)	764.5227	764.5236	$C_{43}H_{76}NO_8P$	$[M-H]^-$	140/281/303/478	1	Negative
71	PE (38:6)	762.5073	762.5079	$C_{43}H_{74}NO_8P$	$[M-H]^-$	140/153/279/303/476	1	Negative
72	PE (40:4)	794.5720	794.5705	$C_{45}H_{82}NO_8P$	$[M-H]^-$	153/283/331	2	Negative
73	PE (40:5)	792.5570	792.5549	$C_{45}H_{80}NO_8P$	$[M-H]^-$	153/283/285/329/480		Negative
74	PE (40:6)	790.5416	790.5392	$C_{45}H_{78}NO_8P$	$[M-H]^-$	153/281/329	3	Negative
75	PE (40:7)	770.5138	770.5125	$C_{45}H_{76}NO_8P$	$[M-H_2O-H]^-$	153/281/283/327/524	2	Negative
76	PE (40:7)	788.5261	788.5236	$C_{45}H_{76}NO_8P$	$[M-H]^-$	153/281/283/327/524	3	Negative
77	PE (40:8)	786.5090	786.5079	$C_{45}H_{74}NO_8P$	$[M-H]^-$	153/279/327	1	Negative
78	PE (42:8)	814.5404	814.5392	$C_{47}H_{78}NO_8P$	$[M-H]^-$	285/305/329	2	Negative
79	PE (42:9)	812.5240	812.5236	$C_{47}H_{76}NO_8P$	$[M-H]^-$	153/303/329/508	0	Negative
80	PE (P-36:4)	722.5150	722.5130	$C_{41}H_{74}NO_7P$	$[M-H]^-$	153/303/418/436	3	Negative
81	PE (P-38:6)	746.5155	746.5130	$C_{43}H_{74}NO_7P$	$[M-H]^-$	283/327/436	3	Negative
82	PE (P-40:6)	774.5473	774.5443	$C_{45}H_{78}NO_7P$	$[M-H]^-$	140/329/444/462	4	Negative

83	PE (P-40:7)	772.5310	772.5287	$C_{45}H_{76}NO_7P$	$[M-H]^-$	283/327/444	3	Negative
84	PE (40:5)	792.5570	792.5549	$C_{45}H_{80}NO_8P$	$[M-H]^-$	153/283/329	3	Negative
85	PE-NMe (36:3)	736.5299	736.5281	$C_{42}H_{78}NO_8P$	$[M-H_2O-H]^-$	140/153/279/281	3	Negative
86	PE-NMe (38:4)	780.5561	780.5549	$C_{44}H_{80}NO_8P$	$[M-H]^-$	153/283/303	2	Negative
87	PE-NMe (38:5)	760.5312	760.5281	$C_{44}H_{78}NO_8P$	$[M-H_2O-H]^-$	153/281/303	4	Negative
88	PE-NMe (38:6)	758.5130	758.5125	$C_{44}H_{76}NO_8P$	$[M-H_2O-H]^-$	153/255/327	1	Negative
89	PE-NMe (40:6)	804.5570	804.5549	$C_{46}H_{80}NO_8P$	$[M-H]^-$	153/283/327	3	Negative
90	PE-NMe (40:7)	802.5422	802.5392	$C_{46}H_{78}NO_8P$	$[M-H]^-$	153/283/325	4	Negative
91	PE-NMe2(40:7)	816.5552	816.5549	$C_{47}H_{80}NO_8P$	$[M-H]^-$	153/281/327	3	Negative
92	PG (34:0)	749.5335	749.5338	$C_{40}H_{79}O_{10}P$	$[M-H]^-$	153/255/283/419/437	0	Negative
93	PG (34:1)	747.5167	747.5182	$C_{40}H_{77}O_{10}P$	$[M-H]^-$	255/281/417/483/491	2	Negative
94	PG (36:0)	777.5646	777.5651	$C_{42}H_{83}O_{10}P$	$[M-H]^-$	153/283/419	0	Negative
95	PG (36:1)	775.5499	775.5495	$C_{42}H_{81}O_{10}P$	$[M-H]^-$	153/281/283	0	Negative
96	PG (36:2)	773.5338	773.5338	$C_{42}H_{79}O_{10}P$	$[M-H]^-$	153/279/283	0	Negative
97	PG (36:3)	771.5158	771.5182	$C_{42}H_{77}O_{10}P$	$[M-H]^-$	279/283/281/153	3	Negative
98	PG (42:8)	845.5351	845.5338	$C_{48}H_{79}O_{10}P$	$[M-H]^-$	153/305/329	2	Negative
99	PG (42:9)	843.5187	843.5182	$C_{48}H_{77}O_{10}P$	$[M-H]^-$	153/303/329	1	Negative

100	PG (44:9)	871.5458	871.5495	$C_{50}H_{81}O_{10}P$	$[M-H]^-$	153/329/331	4	Negative
101	PG (44:10)	869.5363	869.5388	$C_{50}H_{79}O_{10}P$	$[M-H]^-$	153/283/329/419/437	3	Negative
102	PG (44:11)	867.5182	867.5182	$C_{50}H_{77}O_{10}P$	$[M-H]^-$	283/327/329/537/557	0	Negative
103	PI (34:2)	833.5160	833.5186	$C_{43}H_{79}O_{13}P$	$[M-H]^-$	153/241/253/281	3	Negative
104	PI (36:2)	861.5537	861.5499	$C_{45}H_{83}O_{13}P$	$[M-H]^-$	153/241/281/417/579	4	Negative
105	PI (36:3)	859.5340	859.5342	$C_{45}H_{81}O_{13}P$	$[M-H]^-$	153/241/255/305/553	0	Negative
106	PI (36:4)	857.5179	857.5186	$C_{45}H_{79}O_{13}P$	$[M-H]^-$	153/241/255/303/391/553	1	Negative
107	PI (36:4; O)	873.5137	873.5135	$C_{45}H_{79}O_{14}P$	$[M-H]^-$	153/241/255/329	0	Negative
108	PI (38:3)	887.5619	887.5655	$C_{47}H_{85}O_{13}P$	$[M-H]^-$	153/241/283/305/419/581	4	Negative
109	PI (38:3; O)	903.5540	903.5604	$C_{47}H_{85}O_{14}P$	$[M-H]^-$	153/241/283/321/419	6	Negative
110	PI (38:4)	885.5510	885.5499	$C_{47}H_{83}O_{13}P$	$[M-H]^-$	153/241/283/303/437/581	2	Negative
111	PI (38:4; O)	901.5445	901.5448	$C_{47}H_{83}O_{14}P$	$[M-H]^-$	153/241/283/419	0	Negative
112	PI (38:5)	883.5348	883.5342	$C_{47}H_{81}O_{13}P$	$[M-H]^-$	153/241/281/303/417/579	1	Negative
113	PI (38:6)	881.5183	881.5186	$C_{47}H_{79}O_{13}P$	$[M-H]^-$	153 /241/279/303	0	Negative
114	PI (40:5)	911.5678	911.5655	$C_{49}H_{85}O_{13}P$	$[M-H]^-$	153/241/283/329/581	3	Negative
115	PI (40:6)	909.5484	909.5499	$C_{49}H_{83}O_{13}P$	$[M-H]^-$	241/283/327/419/581	2	Negative
116	PI (40:7)	907.5343	907.5342	$C_{49}H_{81}O_{13}P$	$[M-H]^-$	223/241/283/325/625	0	Negative

117	PS (36:2)	786.5299	786.5291	$C_{42}H_{78}NO_{10}P$	$[M-H]^-$	153/279/283/419/437	1	Negative
118	PS (36:3)	784.5124	784.5134	$C_{42}H_{76}NO_{10}P$	$[M-H]^-$	153/279/281/417	1	Negative
119	PS (38:2)	796.5500	796.5492	$C_{44}H_{82}NO_{10}P$	$[M-H_2O-H]^-$	153/283/307	1	Negative
120	PS (38:3)	812.5444	812.5447	$C_{44}H_{80}NO_{10}P$	$[M-H]^-$	153/283/305/419	0	Negative
121	PS (38:4)	810.5310	810.5291	$C_{44}H_{78}NO_{10}P$	$[M-H]^-$	153/283/303/419/437	3	Negative
122	PS (38:5)	808.5143	808.5134	$C_{44}H_{76}NO_{10}P$	$[M-H]^-$	153/255/329/391	1	Negative
123	PS (38:6)	806.4996	806.4978	$C_{44}H_{74}NO_{10}P$	$[M-H]^-$	153/255/327/391	2	Negative
124	PS (40:4)	820.5515	820.5492	$C_{46}H_{82}NO_{10}P$	$[M-H_2O-H]^-$	153/283/331/419	3	Negative
125	PS (40:4)	838.5629	838.5604	$C_{46}H_{82}NO_{10}P$	$[M-H]^-$	153/283/331/419	3	Negative
126	PS (40:4; O)	854.5559	854.5553	$C_{46}H_{82}NO_{11}P$	$[M-H]^-$	153/299/331	1	Negative
127	PS (40:5)	836.5468	836.5453	$C_{46}H_{80}NO_{10}P$	$[M-H]^-$	153/283/329/419/437	2	Negative
128	PS (40:6)	834.5310	834.5291	$C_{46}H_{78}NO_{10}P$	$[M-H]^-$	153/283/327/437	3	Negative
129	PS (40:7)	832.5117	832.5134	$C_{46}H_{76}NO_{10}P$	$[M-H]^-$	153/303/305	2	Negative
130	PS (P-40:6)	818.5348	818.5342	$C_{46}H_{78}NO_9P$	$[M-H]^-$	153/285/329	0	Negative

Table S2 Differential phospholipid signals in the liver sample of Nile tilapia exposed to PFOA compared to control group.

Tissue	Differential ions	Detection mode	Compound name	VIP value	p-value
Liver	754.5374	Positive	PC (34:4)	2.47	9.85E-16
	756.5546	Positive	PC (34:3)	2.49	2.65E-13
	778.5371	Positive	PC (36:6)	3.21	1.29E-21
	780.5528	Positive	PC (36:5)	2.58	2.36E-08
	782.5688	Positive	PC (36:4)	3.09	5.64E-12
	802.5354	Positive	PC (38:8)	2.20	6.78E-15
	804.5506	Positive	PC (38:7)	3.19	2.01E-10
	822.5399	Positive	PC (36:3)	3.07	4.65E-10
	824.5543	Positive	PC (36:2)	2.91	9.32E-12
	828.5521	Positive	PC (40:9)	2.59	6.92E-07
	870.5419	Positive	PC (40:7)	2.10	7.60E-13
	872.5576	Positive	PC (40:6)	2.46	8.18E-15
	874.5740	Positive	PC (40:5)	2.40	9.50E-17
	826.5601	Negative	PS (39:3)	2.02	0.0197
	834.5310	Negative	PS (40:6)	2.16	2.44E-06
	836.5468	Negative	PS (40:5)	3.05	1.41E-04
	851.5820	Negative	PG (42:5)	2.02	3.07E-07
	867.5182	Negative	PG (44:11)	3.47	4.18E-09
	869.5363	Negative	PG (44:10)	6.18	4.23E-06

Table S3 Differential phospholipid signals in the spleen sample of Nile tilapia exposed to PFOA compared to control group.

Tissue	Differential ions	Detection mode	Compound name	VIP value	p-value
Spleen	725.5564	Positive	SM (d36:4)	2.11	1.19E-09
	741.5320	Positive	SM (d34:1)	3.40	3.66E-10
	756.5546	Positive	PC (34:3)	2.01	0.005732
	772.5272	Positive	PC (32:0)	4.79	3.03E-09
	820.5253	Positive	PC (36:4)	3.85	3.21E-11
	828.5521	Positive	PC (40:9)	2.12	1.34E-06
	844.5246	Positive	PC (38:6)	3.43	1.07E-09
	738.5073	Negative	PE (36:4)	2.46	2.38E-08
	746.5155	Negative	PE (P-38:6)	2.10	7.76E-04
	762.5073	Negative	PE (38:6)	3.04	2.81E-10
	766.5395	Negative	PE (38:4)	2.48	1.02E-04
	836.5468	Negative	PS (40:5)	2.07	4.85E-04
	843.5187	Negative	PG (42:9)	2.33	1.55E-06
	845.5351	Negative	PG (42:8)	2.08	2.70E-07
	861.5537	Negative	PI (36:2)	2.10	1.40E-08
	867.5182	Negative	PG (44:11)	5.29	1.46E-06
	869.5363	Negative	PG (44:10)	6.03	2.71E-09
	871.5458	Negative	PG (44:9)	4.59	8.05E-09