Table S1. Matrix of data used for the unsupervised PCA

Sample	PE/LPE[a]	PC/LPC[a]	PC/PE[a]	PC/SM[a]
F_GR	3.9	5.0	6.6	24.5
F_TAf1	6.1	69.4	14.6	35.5
F_TAf2	9.3	112.4	14.7	30.8
F_TAf3	8.0	73.5	15.2	38.2
F_TA1	4.3	7.6	7.3	30.4
F_TA2	2.0	6.1	12.4	10.3
F_TA3	2.1	6.0	12.5	25.7
F_TA4	3.2	9.8	11.6	25.1
F_TA5	4.5	11.0	12.7	34.9
F_TR1	1.5	6.1	12.2	36.8
F_TR2	0.8	1.6	5.2	30.3
F_TR3	0.9	1.4	4.4	23.7
F_TR4	1.0	3.4	12.1	30.0
F_ME	1.2	1.5	7.6	15.9
W_ME	2.1	11.5	16.1	21.2
W_BR	4.4	39.9	14.8	32.9

[a] Ratios of the integrated areas obtained for class-related bands in the HILIC-ESI(+)-FTMS chromatogram

Table S2. Overview of PEs identified by HILIC-ESI-FTMS in positive ion mode. All polar lipids were extracted from fillets of wild and farmed *S. aurata*

ID	Exact Mass	Accurate Mass (wild)	Accuracy (ppm)	Accurate Mass (farmed)	Accuracy (ppm)	Lipid species	Adduct	Sum Formula
PE_1	674.5119	674.5124	0.72	674.5125	0.86	PE O-32:2	H+	C37H73NO7P
PE_2	688.5276	688.5281	0.77	688.5286	1.50	PE O-33:2	H+	C38H75NO7P
PE_3	700.5276	700.5278	0.33	700.5284	1.19	PE O-34:3	H+	C39H75NO7P
PE_4	702.5432	702.5437	0.69	702.5448	2.25	PE O-34:2	H+	C39H77NO7P
PE_5	714.5068	-	-	714.5079	1.50	PE 34:3	H+	C39H73NO8P
PE_6	714.5432	714.5435	0.40	714.5441	1.24	PE O-35:3	H+	C40H77NO7P
PE_7	716.5225	716.5236	1.56	716.5234	1.28	PE 34:2	H+	C39H75NO8P
PE_8	716.5589	716.5593	0.60	716.5602	1.86	PE O-35:2	H+	C40H79NO7P
PE_9	718.5381	718.5388	0.93	718.5399	2.46	PE 34:1	H+	C39H77NO8P
PE_10	722.5119	722.5121	0.25	722.5129	1.36	PE O-36:6	H+	C41H73NO7P
PE_11	724.5276	724.5277	0.18	724.5278	0.32	PE O-36:5	H+	C41H75NO7P
PE_12	726.5432	726.5445	1.77	726.5443	1.49	PE O-36:4	H+	C41H77NO7P
PE_13	728.5589	728.5591	0.32	728.5600	1.56	PE O-36:3	H+	C41H79NO7P
PE_14	730.5745	730.5752	0.93	730.5762	2.30	PE O-36:2	H+	C41H81NO7P
PE_15	734.5119	734.5119	-0.02	734.5128	1.20	PC O-34:7	H+	C42H73NO7P
PE_16	738.5068	738.5071	0.36	738.5076	1.04	PE 36:5	H+	C41H73NO8P
PE_17	738.5432	738.5432	-0.02	-	-	PE O-37:5	H+	C42H77NO7P
PE_18	740.5225	740.5227	0.30	740.5236	1.51	PE 36:4	H+	C41H75NO8P
PE_19	742.5381	-	-	742.5391	1.30	PE 36:3	H+	C41H77NO8P
PE_20	744.5538	744.5543	0.70	744.5547	1.23	PE 36:2	H+	C41H79NO8P
PE_21	746.5694	-	-	746.5706	1.56	PE 36:1	H+	C41H81NO8P
PE_22	746.5119	746.5121	0.25	746.5128	1.18	PE O-38:8	H+	C43H73NO7P
PE_23	748.5276	748.5278	0.31	748.5282	0.85	PE O-38:7	H+	C43H75NO7P
PE_24	750.5432	750.5437	0.64	750.5445	1.71	PE O-38:6	H+	C43H77NO7P
PE_25	752.5589	752.5592	0.44	752.5595	0.84	PE O-38:5	H+	C43H79NO7P
PE_26	754.5381	754.5381	-0.04	-	-	PE 37:4	H+	C42H77NO8P
PE_27	760.5276	760.5268	-1.01	-	-	PE O-39:8	H+	C44H75NO7P
PE_28	762.5068	762.5058	-1.35	762.5078	1.27	PE 38:7	H+	C43H73NO8P
PE_29	762.5432	762.5427	-0.68	762.5437	0.63	PE O-39:7	H+	C44H77NO7P
PE_30	764.5225	764.5222	-0.37	764.5235	1.33	PE 38:6	H+	C43H75NO8P
PE_31	764.5589	764.5583	-0.74	-	-	PE O-39:6	H+	C44H79NO7P
PE_32	766.5381	766.5389	1.00	766.5391	1.26	PE 38:5	H+	C43H77NO8P
PE_33	768.5538	768.5534	-0.50	768.5554	2.11	PE 38:4	H+	C43H79NO8P
PE_34	770.5119	770.5092	-3.53	770.5114	-0.67	PE O-40:10	H+	C45H73NO7P
PE_35	770.5694	770.5688	-0.82	770.5705	1.39	PE 38:3	H+	C43H81NO8P
PE_36	772.5276	772.5272	-0.48	772.5282	0.82	PE O-40:9	H+	C45H75NO7P
PE_37	774.5432	774.5426	-0.80	774.5442	1.27	PE O-40:8	H+	C45H77NO7P
PE_38	776.5589	776.5583	-0.73	776.56	1.46	PE O-40:7	H+	C45H79NO7P
PE_39	778.5381	778.5373	-1.07	778.5384	0.35	PE 39:6	H+	C44H77NO8P
PE_40	778.5745	778.5724	-2.72	-	-	PE O-40:6	H+	C45H81NO7P
PE_41	780.5902	780.5907	0.68	-	-	PE O-40:5	H+	C45H83NO7P
PE_42	782.5694	782.5689	-0.68	-	-	PE 39:4	H+	C44H81NO8P
PE_43	786.5068	786.5045	-2.96	786.5069	0.09	PE 40:9	H+	C45H73NO8P
PE_44	788.5225	788.5213	-1.50	788.5235	1.29	PE 40:8	H+	C45H75NO8P
PE_45	788.5589	788.5577	-1.48	-	-	PE O-41:8	H+	C46H79NO7P

PE_46	790.5381	790.5372	-1.18	790.5383	0.21	PE 40:7	H+	C45H77NO8P
PE_47	790.5745	790.5732	-1.67	-	-	PE O-41:7	H+	C46H81NO7P
PE_48	792.5538	792.553	-0.99	792.5529	-1.11	PE 40:6	H+	C45H79NO8P
PE_49	794.5694	794.5678	-2.05	-	-	PE 40:5	H+	C45H81NO8P
PE_50	796.5851	796.5849	-0.23	796.5841	-1.23	PE 40:4	H+	C45H83NO8P
PE_51	798.5432	-	-	798.5414	-2.28	PE O-42:10	H+	C47H77NO7P
PE_52	798.6007	798.6008	0.09	798.6011	0.46	PE 40:3	H+	C45H85NO8P
PE_53	802.5745	802.5736	-1.14	802.5746	0.10	PE O-42:8	H+	C47H81NO7P
PE_54	806.5330	-	-	806.5329	-0.18	NAPE 40:6	H+	C45H77NO9P
PE_55	806.5694	806.5683	-1.40	806.5687	-0.91	PE 41:6	H+	C46H81NO8P
PE_56	810.5068	810.5057	-1.40	810.5064	-0.53	PE 42:11	H+	C47H73NO8P
PE_57	812.5225	812.5215	-1.21	812.5221	-0.47	PE 42:10	H+	C47H75NO8P
PE_58	814.5381	-	-	814.5369	-1.51	PE 42:9	H+	C47H77NO8P
PE_59	816.5538	816.5535	-0.35	816.5544	0.76	PE 42:8	H+	C47H79NO8P
PE_60	818.5694	818.5685	-1.14	818.5695	0.08	PE 42:7	H+	C47H81NO8P
PE_61	820.5851	-	-	820.5855	0.51	PE 42:6	H+	C47H83NO8P
PE_62	836.5225	836.5218	-0.81	836.5237	1.46	DMPE 42:12[f]	H+	C49H75NO8P
PE_63	838.5381	838.5365	-1.95	838.5381	-0.04	DMPE 42:11[f]	H+	C49H77NO8P
PE_64	840.5538	840.5535	-0.34	-	-	DMPE 42:10[f]	H+	C49H79NO8P
PE_65	858.5044	858.5031	-1.54	858.5048	0.44	DMPE 42:12[f]	Na+	C49H74NO8PNa

[a] Monoisotopic exact mass was calculated by using the online lipid calculator (see text). **[b]** Experimental value of positively charged molecules. **[c]** Error expressed in parts per million (ppm) and evaluated as 10^6 x (accurate mass – exact mass)/accurate mass. **[d]** Lipid species were annotated as follows: PL <M carbon atoms in acyl chains>:<N double bonds in acyl chains>. **[e]** Ether species were annotated with the general notation recently proposed (PE O-), even if some of them might correspond mainly to vinyl ether species (for which a PE P- notation should be used). **[f]** Although only N,N-dimethyl-PE (DMPE) were obtained as possible candidates after lipid database searching based on the reported *m/z* values, the latter might also be related to PE with two further carbon atoms on their acyl chains, not listed in the databases. Note: NAPE 40:6 is a N-acyl-PE

Table S3. Overview of LPEs identified by HILIC-ESI-FTMS in positive ion mode

ID	Exact Mass	Accurate Mass (wild)	Accuracy (ppm)	Accurate Mass (farmed)	Accuracy (ppm)	Lipid species	Adduct	Sum Formula
LPE_1	438.2979	438.2978	-0.23	438.2980	0.23	LPE O-16:1	H^+	C21H45NO6P
LPE_2	452.3136	452.3134	-0.33	-	-	LPE O-17:1	H^+	C22H47NO6P
LPE_3	454.2928	454.2927	-0.26	454.2932	0.85	LPE 16:0	H^+	C21H45NO7P
LPE_4	462.2979	462.2978	-0.22	462.2980	0.21	LPE O-18:3	H^+	C23H45NO6P
LPE_5	464.3136	464.3135	-0.11	464.3138	0.54	LPE O-18:2	H^+	C23H47NO6P
LPE_6	466.2928	466.2928	-0.03	466.2932	0.82	LPE 17:1	H^+	C22H45NO7P
LPE_7	466.3292	466.3291	-0.22	466.3293	0.21	LPE O-18:1	H^+	C23H49NO6P
LPE_8	468.3085	468.3085	0.07	468.3091	1.35	LPE 17:0	H^+	C22H47NO7P
LPE_9	476.2772	-	-	476.2772	0.07	LPE 18:3	H^+	C23H43NO7P
LPE_10	478.2928	478.2929	0.18	478.2932	0.80	LPE 18:2	H^+	C23H45NO7P
LPE_11	480.3085	480.3084	-0.14	480.3088	0.70	LPE 18:1	H^+	C23H47NO7P
LPE_12	482.3241	482.3241	-0.03	482.3242	0.17	LPE 18:0	H^+	C23H49NO7P
LPE_13	496.3398	496.3397	-0.13	496.3401	0.67	LPE 19:0	H^+	C24H51NO7P
LPE_14	500.2772	500.2770	-0.33	500.2771	-0.13	LPE 20:5	H^+	C25H43NO7P
LPE_15	502.2928	502.2927	-0.23	502.2926	-0.43	LPE 20:4	H^+	C25H45NO7P
LPE_16	504.3085	-	-	504.3076	-1.72	LPE 20:3	H^+	C25H47NO7P
LPE_17	506.3241	506.3243	0.36	506.3245	0.76	LPE 20:2	H^+	C25H49NO7P
LPE_18	508.2798	-	-	-	-	LPE O-20:5	Na+	C25H44NO6PNa
LPE_19	508.3398	508.3400	0.46	508.3401	0.66	LPE 20:1	H^+	C25H51NO7P
LPE_20	510.3554	510.3546	-1.60	510.3559	0.95	LPE 20:0	H^+	C25H53NO7P
LPE_21	514.2928	-	-	514.2934	1.14	LPE 21:5	H^+	C26H45NO7P
LPE_22	522.2591	-	-	522.2599	1.51	LPE 20:5	Na+	C25H42NO7PNa
LPE_23	524.2748	524.2754	1.22	-	-	LPE 20:4	Na^+	C25H44NO7PNa
LPE_24	526.2928	526.2928	-0.03	526.2933	0.92	LPE 22:6	H^+	C27H45NO7P
LPE_25	528.3085	528.3084	-0.12	528.3078	-1.26	LPE 22:5	H^+	C27H47NO7P
LPE_26	530.3241	530.3240	-0.22	530.3236	-0.97	LPE 22:4	H^+	C27H49NO7P
LPE_27	548.2748	548.2748	0.07	548.2747	-0.11	LPE 22:6	H^+	C27H44NO7PNa

[a] Monoisotopic exact mass was calculated by using the online lipid calculator (see text). [b] Experimental value of positively charged molecules. [c] Error expressed in parts per million (ppm) and evaluated as 10^6 x (accurate mass – exact mass)/accurate mass. [d] Lipid species were annotated as follows: PL <M carbon atoms in acyl chains>:<N double bonds in acyl chains>. [e] Ether species were annotated using the general nomenclature recently proposed for these lipids (O-)

Table S4. Overview of PCs identified by HILIC-ESI-FTMS in positive ion mode

ID	Exact Mass	Accurate Mass (Wild)	Accuracy (ppm)	Accurate Mass (Farmed)	Accuracy (ppm)	Lipid species	Adduct	Sum Formula
PC_1	718.5745	718.5752	0.95	718.5757	1.65	PC O-32:1	H+	C40H81NO7P
PC_2	730.5381	730.5398	2.28	-	-	PC 32:2	H+	C40H77NO8P
PC_3	732.5538	732.5549	1.53	732.5556	2.48	PC 32:1	H+	C40H79NO8P
PC_4	734.5694	734.569	-0.59	734.5699	0.64	PC 32:0	H+	C40H81NO8P
PC_5	738.5432	738.5437	0.65	738.5438	0.79	PC O-34:5	H+	C42H77NO7P
PC_6	744.5902	744.5911	1.25	744.5911	1.25	PC O-34:2	H+	C42H83NO7P
PC_7	746.5694	746.5706	1.56	-	-	PC 33:1	H+	C41H81NO8P
PC_8	746.6058	746.6046	-1.63	746.6061	0.38	PC O-34:1	H+	C42H85NO7P
PC_9	752.5589	752.5589	0.04	752.5600	1.51	PC O-35:5	H+	C43H79NO7P
PC_10	754.5381	754.539	1.15	754.5390	1.15	PC 34:4	H+	C42H77NO8P
PC_11	756.5538	756.5538	0.02	756.5554	2.14	PC 34:3	H+	C42H79NO8P
PC_12	758.5694	758.5702	1.01	758.5699	0.62	PC 34:2	H+	C42H81NO8P
PC_13	760.5851	760.5843	-1.03	760.5833	-2.34	PC 34:1	H+	C42H83NO8P
PC_14	762.5432	762.5439	0.90	762.5446	1.81	PC O-36:7	H+	C44H77NO7P
PC_15	764.5589	764.5593	0.57	764.5603	1.87	PC O-36:6	H+	C44H79NO7P
PC_16	766.5745	766.5749	0.50	766.5760	1.93	PC O-36:5	H+	C44H81NO7P
PC_17	768.5538	768.5547	1.19	768.5554	2.11	PC 35:4	H+	C43H79NO8P
PC_18	768.5902	768.5889	-1.65	-	-	PC O-36:4	H+	C44H83NO7P
PC_19	770.5694	770.5679	-1.99	770.5693	-0.17	PC 35:3	H+	C43H81NO8P
PC_20	772.5851	772.5843	-1.01	772.5858	0.93	PC 35:2	H+	C43H83NO8P
PC_21	774.6007	774.5994	-1.72	774.6007	-0.04	PC 35:1	H+	C43H85NO8P
PC_22	776.5589	776.5589	0.04	-	-	PC O-37:7	H+	C45H79NO7P
PC_23	778.5381	778.5395	1.76	778.5384	0.35	PC 36:6	H+	C44H77NO8P
PC_24	778.5745	778.5748	0.36	-	-	PC O-37:6	H+	C45H81NO7P
PC_25	780.5538	780.5542	0.54	780.5533	-0.62	PC 36:5	H+	C44H79NO8P
PC_26	780.5902	780.5903	0.17	-	-	PC O-37:5	H+	C45H83NO7P
PC_27	782.5694	782.5683	-1.45	782.5694	-0.04	PC 36:4	H+	C44H81NO8P
PC_28	784.5851	-	-	784.5846	-0.61	PC 36:3	H+	C44H83NO8P
PC_29	786.6007	786.5996	-1.44	786.5987	-2.58	PC 36:2	H+	C44H85NO8P
PC_30	788.5589	788.5583	-0.72	-	-	PC O-38:8	H+	C46H79NO7P
PC_31	788.6164	788.6153	-1.37	788.6140	-3.02	PC 36:1	H+	C44H87NO8P
PC_32	790.5745	790.5751	0.74	790.5755	1.24	PC O-38:7	H+	C46H81NO7P
PC_33	792.5538	792.5525	-1.62	792.5547	1.16	PC 37:6	H+	C45H79NO8P
PC_34	792.5902	792.5879	-2.86	792.5903	0.17	PC O-38:6	H+	C46H83NO7P
PC_35	794.5694	794.569	-0.54	794.5686	-1.05	PC 37:5	H+	C45H81NO8P
PC_36	794.6058	794.6055	-0.40	-	-	PC O-38:5	H+	C46H85NO7P
PC_37	796.5851	796.5848	-0.35	796.5857	0.78	PC 37:4	H+	C45H83NO8P
PC_38	802.5381	-	-	802.5369	-1.53	PC 38:8	H+	C46H77NO8P
PC_39	804.5538	804.5521	-2.09	804.5549	1.39	PC 38:7	H+	C46H79NO8P
PC_40	804.5902	804.5896	-0.70	804.5913	1.41	PC O-39:7	H+	C47H83NO7P
PC_41	806.5694	806.5682	-1.53	806.5692	-0.29	PC 38:6	H+	C46H81NO8P
PC_42	812.6140	-	-	812.6149	1.14	PC 36:0	+Na+	C44H88NO8PNa

PC_43	814.6320	814.6305	-1.88	814.6309	-1.39	PC 38:2	H+	C46H89NO8P
PC_44	816.5902	816.5902	0.04	816.5915	1.63	PC O-40:8	H+	C48H83NO7P
PC_45	818.5694	818.5677	-2.12	818.5696	0.21	PC 39:7	H+	C47H81NO8P
PC_46	818.6058	818.6054	-0.51	818.6055	-0.39	PC O-40:7	H+	C48H85NO7P
PC_47	820.5252	820.5228	-2.88	-	-	PC O-39:10	+Na+	C47H76NO7PNa
PC_48	820.5851	820.5832	-2.29	820.5836	-1.81	PC 39:6	H+	C47H83NO8P
PC_49	822.6007	822.5997	-1.25	822.6007	-0.04	PC 39:5	H+	C47H85NO8P
PC_50	830.5694	830.5687	-0.88	830.5694	-0.04	PC 40:8	H+	C48H81NO8P
PC_51	832.5851	832.5834	-2.02	832.5839	-1.42	PC 40:7	H+	C48H83NO8P
PC_52	852.5538	852.5545	0.84	852.5537	-0.10	PC 42:11	H+	C50H79NO8P
PC_53	854.5694	854.5686	-0.97	-	-	PC 42:10	H+	C50H81NO8P
PC_54	856.5851	-	-	856.5832	-2.20	PC 42:9	H+	C50H83NO8P
PC_55	858.6007	858.5985	-2.60	858.5995	-1.43	PC 42:8	H+	C50H85NO8P
PC_56	860.6164	-	-	860.6155	-1.02	PC 42:7	H+	C50H87NO8P
PC_57	870.6946	-	-	870.6930	-1.87	PC 42:2	H+	C50H97NO8P
PC_58	872.7103	-	-	872.7080	-2.61	PC 42:1	H+	C50H99NO8P
PC_59	878.5670	878.5690	2.28	878.5697	3.04	PC 42:9	Na+	C50H82NO8PNa
PC_60	880.5827	880.5819	-0.91	880.5830	-0.88	PC 42:8	Na+	C50H84NO8PNa
PC_61	882.5983	882.5983	-0.03	-	-	PC 42:7	Na+	C50H86NO8PNa

[a] Monoisotopic exact mass was calculated by using the online lipid calculator (see text). [b] Experimental value of positively charged molecules. [c] Error expressed in parts per million (ppm) and evaluated as 10^6 x (accurate mass – exact mass)/accurate mass. [d] Lipid species were annotated as follows: PL <M carbon atoms in acyl chains>:<N double bonds in acyl chains>. [e] Ether species were annotated using the general nomenclature recently proposed for these lipids (O-)

Table S5. Overview of LPCs identified by HILIC-ESI-FTMS in positive ion mode

ID	Exact Mass	Accurate Mass (wild)	Accuracy (ppm)	Accurate Mass (farmed)	Accuracy (ppm)	Lipid species	Adduct	Sum Formula
LPC_1	478.3292	478.3291	-0.21	478.3287	-1.05	LPC O-16:2	H^+	C24H49NO6P
LPC_2	480.3449	480.3446	-0.52	480.3445	-0.73	LPC O-16:1	H^+	C24H51NO6P
LPC_3	482.3241	482.3242	0.17	-	-	LPC 15:0	H^+	C23H49NO7P
LPC_4	494.3241	494.3242	0.17	494.3238	-0.64	LPC 16:1	H^+	C24H49NO7P
LPC_5	494.3605	494.3604	-0.20	494.3604	-0.20	LPC O-17:1	H^+	C25H53NO6P
LPC_6	496.3398	496.3395	-0.54	496.3396	-0.33	LPC 16:0	H^+	C24H51NO7P
LPC_7	500.3111	-	-	500.3108	-0.60	LPC O-16:2	Na+	C24H48NO6PNa
LPC_8	502.3268	502.3271		502.3276	1.59	LPC O-16:1	Na+	C24H50NO6PNa
LPC_9	504.3449	-	-	504.3450	0.20	LPC O-18:3	H+	C26H51NO76P
LPC_10	508.3398	508.3396	-0.33	508.3406	1.64	LPC 17:1	H^+	C25H51NO7P
LPC_11	508.3762	508.3763	0.29	508.3757	-0.89	LPC O-18:1	H^+	C26H55NO6P
LPC_12	510.3554	510.3556	0.36	510.3569	2.91	LPC 17:0	H^+	C25H53NO7P
LPC_13	516.3085	516.3074	-2.13	516.3084	-0.19	LPC 18:4	H^+	C26H47NO7P
LPC_14	518.3217	518.3217	-0.02	-	-	LPC 16:0	Na^+	C24H50NO7PNa
LPC_15	520.3398	520.3399	0.26	520.3395	-0.51	LPC 18:2	H^+	C26H51NO7P
LPC_16	522.3554	522.3554	-0.03	522.3551	-0.60	LPC 18:1	H^+	C26H53NO7P
LPC_17	524.3711	524.3711	0.06	524.3711	0.06	LPC 18:0	H^+	C26H55NO7P
LPC_18	540.3061	-	-	540.3062	0.19	LPC 18:3	Na^+	C26H48NO7PNa
LPC_19	542.3241	542.3237	-0.74	542.3237	0.00	LPC 18:2	H^+	C28H49NO7P
LPC_20	544.3398	544.3397	-0.12	544.3393	-0.86	LPC 20:4	H^+	C28H51NO7P
LPC_21	546.3554	546.3548	-1.13	546.3554	-0.03	LPC 20:3	H^+	C28H53NO7P
LPC_22	548.3711	548.3708	-0.49	548.3710	-0.12	LPC 20:2	H^+	C28H55NO7P
LPC_23	550.3268	-	-	550.3274	1.09	LPC O-20:5	Na^+	C28H50NO6PNa
LPC_24	552.4024	-	-	552.4025	0.18	LPC 20:0	H^+	C28H59NO7P
LPC_25	558.3554	558.3555	0.15	558.3566	2.12	LPC 21:4	H^+	C29H53NO7P
LPC_26	564.3061	564.306	-0.11	564.3056	-0.82	LPC 20:5	Na^+	C28H50NO7PNa
LPC_27	566.3217	566.3214	-0.53	566.3212	-0.88	LPC 20:4	Na^+	C28H48NO7PNa
LPC_28	568.3398	568.3396	-0.29	568.3393	-0.82	LPC 22:6	H^+	C30H51NO7P
LPC_29	570.3554	570.3551	-0.55	570.3553	-0.20	LPC 22:5	H^+	C30H53NO7P
LPC_30	572.3711	572.3702	-1.51	572.3708	-0.46	LPC 22:4	H^+	C30H55NO7P
LPC_31	578.4180	578.4181	0.17	578.4180	-0.06	LPC 22:1	H^+	C30H61NO7P
LPC_32	590.3217	590.3211	-1.03	590.3209	-1.37	LPC 22:6	Na^+	C30H50NO7PNa
LPC_33	592.3374	592.3372	-0.27	592.3372	-0.27	LPC 22:5	Na^+	C30H52NO7PNa
LPC_34	594.3530	594.3525	-0.84	594.3528	-0.34	LPC 22:4	Na^+	C30H54NO7PNa

[a] Monoisotopic exact mass was calculated by using the online lipid calculator (see text). [b] Experimental value of positively charged molecules. [c] Error expressed in parts per million (ppm) and evaluated as 10^6 x (accurate mass – exact mass)/accurate mass. [d] Lipid species were annotated as follows: PL <M carbon atoms in acyl chains>:<N double bonds in acyl chains>. [e] Ether species were annotated using the general nomenclature recently proposed for these lipids (O-)

Table S6. Overview of SMs identified by HILIC-ESI-FTMS in positive ion mode.

ID	Exact[a] Mass	Accurate Mass [b](wild)	Accuracy[c] (ppm)	Accurate Mass[b] (farmed)	Accuracy[c] (ppm)	Lipid[d] species	Adduct	Sum Formula
SM_1	675.5436	675.5434	-0.22	675.5442	0.89	SM 32:1;2	+H+	C37H76N2O6P
SM_2	689.5592	689.5590	-0.29	689.5594	0.29	SM 33.1,2	+H+	C38H78N2O6P
SM_3	717.5905	717.5901	-0.56	717.5906	0.14	SM 35:1;2	+H+	C40H82N2O6P
SM_4	703.5749	703.5746	-0.36	703.5755	0.92	SM 34:1;2	+H+	C39H80N2O6P
SM_5	727.5724	727.5745	2.82	727.5735	1.45	SM 34:0;2	+Na+	C39H81N2O6PNa
SM_6	731.6062	731.6058	-0.48	731.6054	-1.03	SM 36:1;2	+H+	C41H84N2O6P
SM_7	741.5881	741.59	2.57	-	-	SM 35:0;2	+Na+	C40H83N2O6PNa
SM_8	755.6037	755.6055	2.32	-	-	SM 36:0;2	+Na+	C41H85N2O6PNa
SM_9	757.6218	757.6215	-0.40	757.6226	1.05	SM 38:2;2	+H+	C43H86N2O6P
SM_10	759.6375	759.6373	-0.20	759.6374	-0.07	SM 38:1;2	+H+	C43H88N2O6P
SM_11	769.6194	769.6214	2.60	-	-	SM 37:0;2	+Na+	C42H87N2O6PNa
SM_12	771.6375	771.6373	-0.20	771.6385	1.36	SM 39:2;2	+H+	C44H88N2O6P
SM_13	781.6194	781.6217	2.95	-	-	SM 38:1;2	+Na+	C43H87N2O6PNa
SM_14	783.6350	783.6372	2.75	-	-	SM 38:0;2	+Na+	C43H89N2O6PNa
SM_15	785.6531	785.6528	-0.38	785.6536	0.63	SM 40:2;2	+H+	C45H90N2O6P
SM_16	795.6350	795.6373	2.83	-	-	SM 39:1;2	+Na+	C44H89N2O6PNa
SM_17	799.6688	799.6686	-0.19	799.6699	1.44	SM 41:2;2	+H+	C46H92N2O6P
SM_18	801.6844	-	-	801.6859	1.87	SM 41:1;2	+H+	C46H94N2O6P
SM_19	807.6350	807.6354	0.44	807.6364	1.68	SM 40:2;2	+Na+	C45H89N2O6PNa
SM_20	811.6663	811.6686	2.78	-	-	SM 40:0;2	+Na+	C45H93N2O6PNa
SM_21	813.6844	813.684	-0.49	813.6848	0.49	SM 42:2;2	+H+	C47H94N2O6P
SM_22	821.6507	821.6525	2.20	821.6518	1.34	SM 41:2;2	+Na+	C46H91N2O6PNa
SM_23	823.6663	823.6681	2.13	823.6687	2.86	SM 41:1;2	+Na+	C46H93N2O6PNa
SM_24	827.7001	827.699	-1.27	827.6989	-1.39	SM 43:2;2	+H+	C48H96N2O6P
SM_25	831.6950	831.6946	-0.44	831.6948	-0.20	SM 42:1;3	+H+	C47H96N2O7P
SM_26	835.6663	835.6653	-1.25	835.6649	-1.73	SM 42:2;2	+Na+	C47H93N2O6PNa
SM_27	837.6820	837.683	1.20	-	-	SM 42:1;2	+Na+	C47H95N2O6PNa
SM_28	841.7157	841.7147	-1.19	841.7151	-0.72	SM 44:2;2	+H+	C49H98N2O6P
SM_29	851.6976	851.6996	2.29	-	-	SM 43:1;2	+Na+	C48H97N2O6PNa

[a] Monoisotopic exact mass was calculated by using the online lipid calculator (see text); **[b]** experimental value of positively charged molecules; **[c]** error expressed in parts per million (ppm) and evaluated as 10^6 x (accurate mass – exact mass)/accurate mass; **[d]** lipid species were annotated as follows: SM <M carbon atoms>:<N double bonds >;<OH index>, where the M number accounts for all carbon atoms but those included in the phosphocholine headgroup

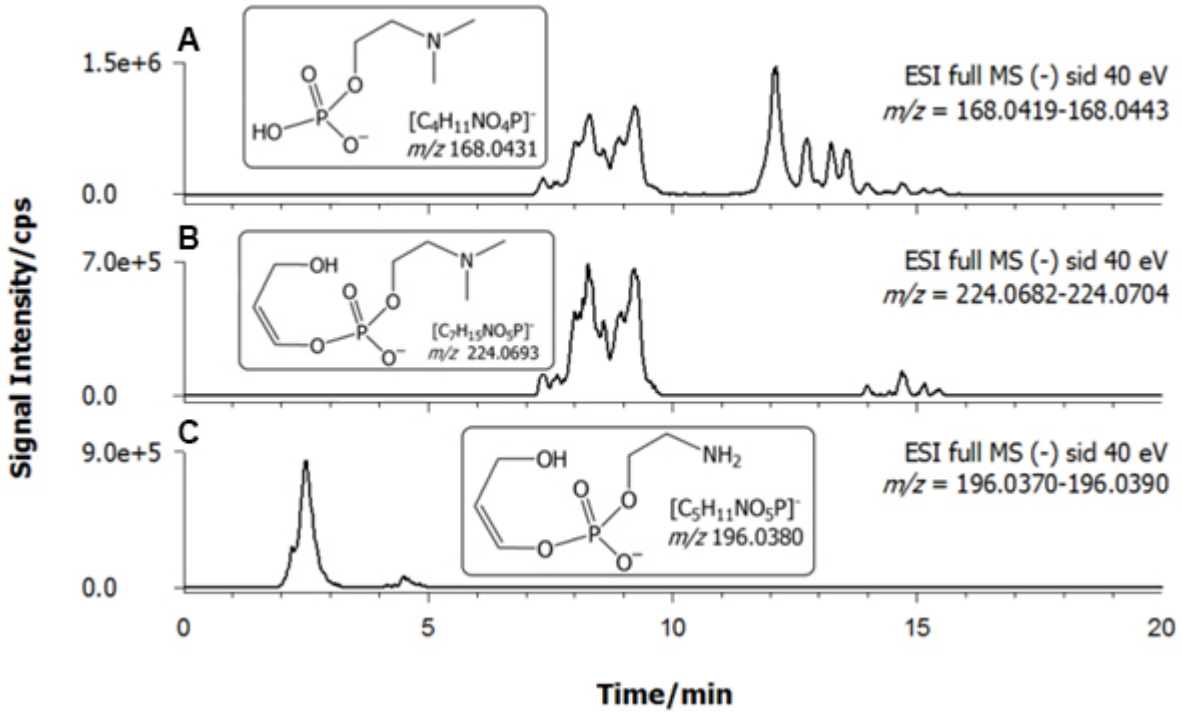

Figure S1. Extracted ion current chromatograms (EIC) obtained by HILIC-ESI(-)-FTMS of phospholipids extracted from fillets of farmed *S. aurata* using the acquisition tool named "all ion fragmentation" (AIF). XIC chromatograms were obtained using narrow windows centred on the selected *m/z* values corresponding to the following class-diagnostic ions: (A) *m/z* 168.0431 (PC, SM and LPC), (B) *m/z* 224.0693 (PC and LPC) and (C) *m/z* 196.0380 (PE and LPE). The ESI-AIF-FTMS spectra were obtained by applying a source-induced dissociation (sid) with a collisional energy of 40 eV and HCD 35%

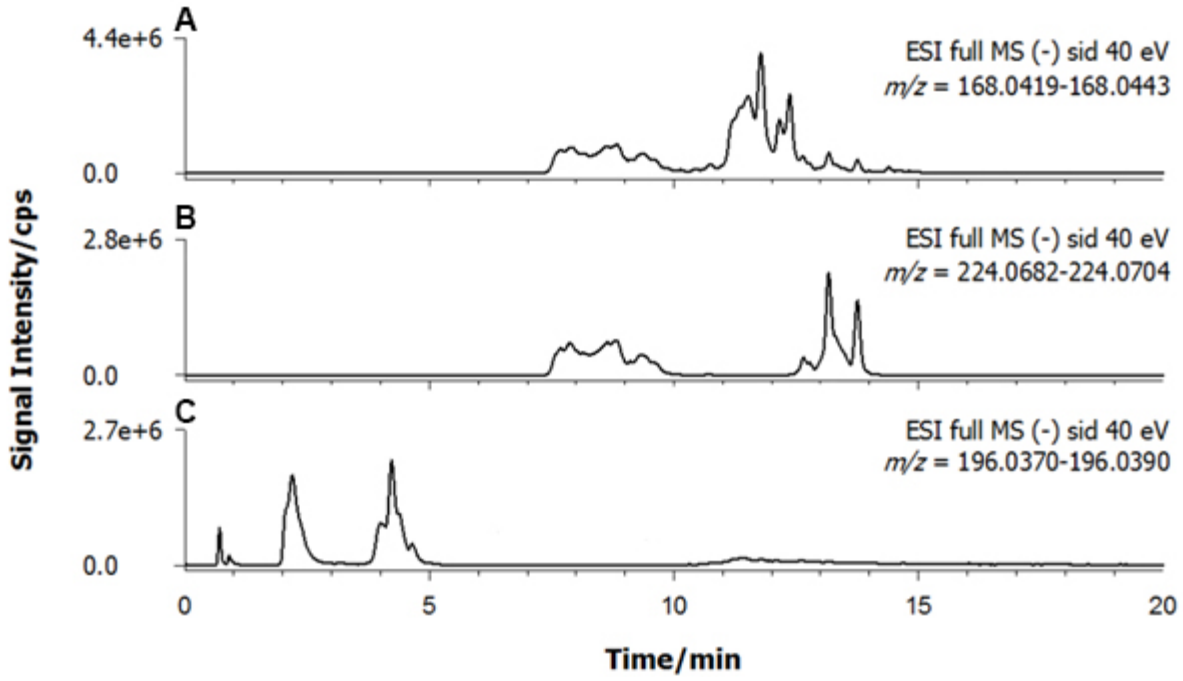

Figure S2. EIC chromatograms obtained by HILIC-ESI(-)-FTMS of phospholipids extracted from fillets of wild *S. aurata* using the AIF acquisition. EIC chromatograms were obtained using narrow windows centred on selected *m/z* values corresponding to the following class diagnostic ions: (A) *m/z* 168.0431 (PC, SM and LPC), (B) *m/z* 224.0693 (PC and LPC) and (C) *m/z* 196.0380 (PE and LPE). The same experimental conditions of Figure S1 were applied

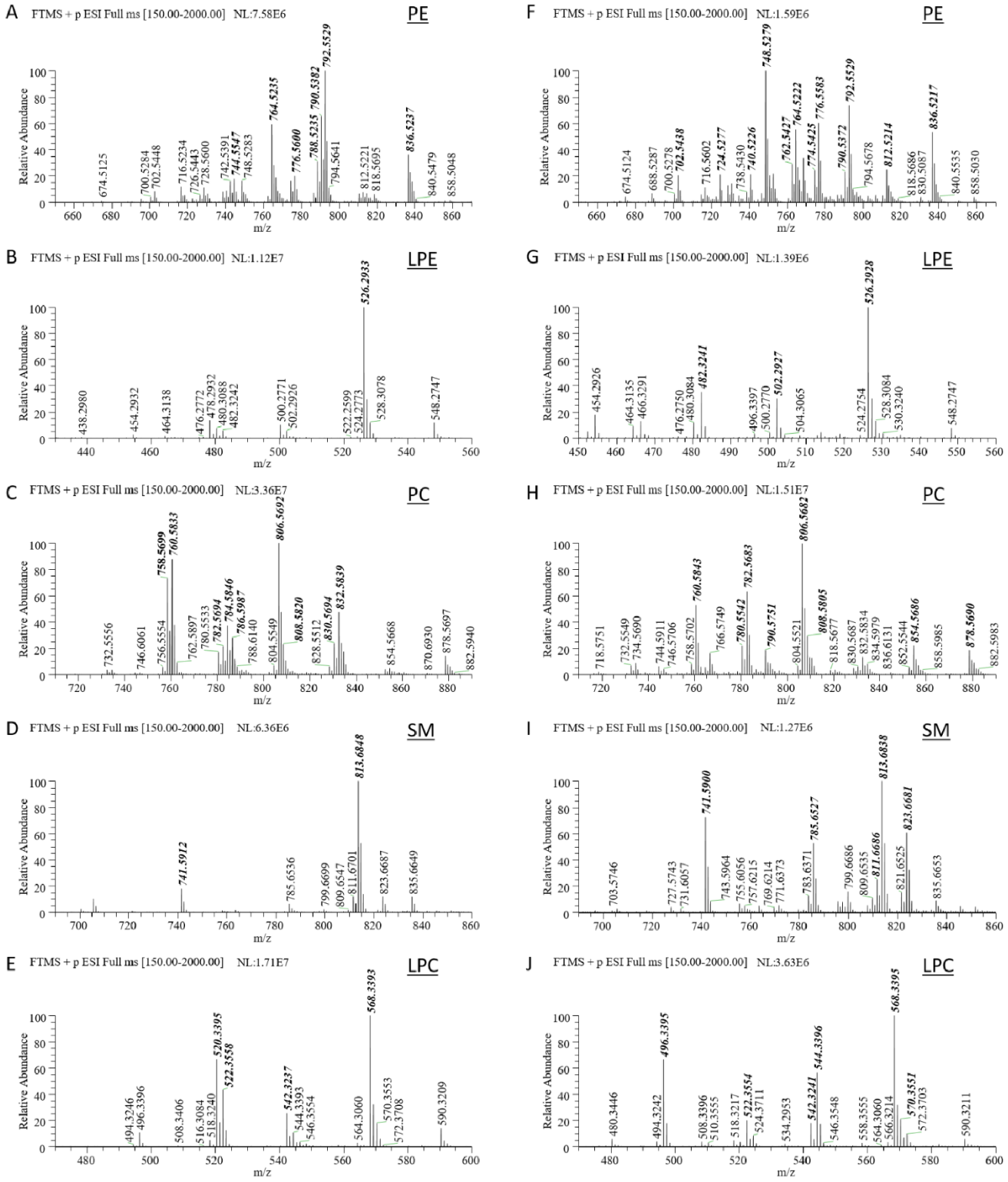

Figure S3. ESI(+)-FTMS spectra of PL classes obtained by averaging the HILIC-ESI(+)-FTMS spectra acquired in the retention times intervals related to each PL band, established as shown in Figure 1. Plots A, B, C, D and E refer to farmed samples, and F, G, H, I and J refer to wild ones. Peak signals labelled with bold *m/z* values correspond to species exhibiting a relative abundance at least equal to 20%

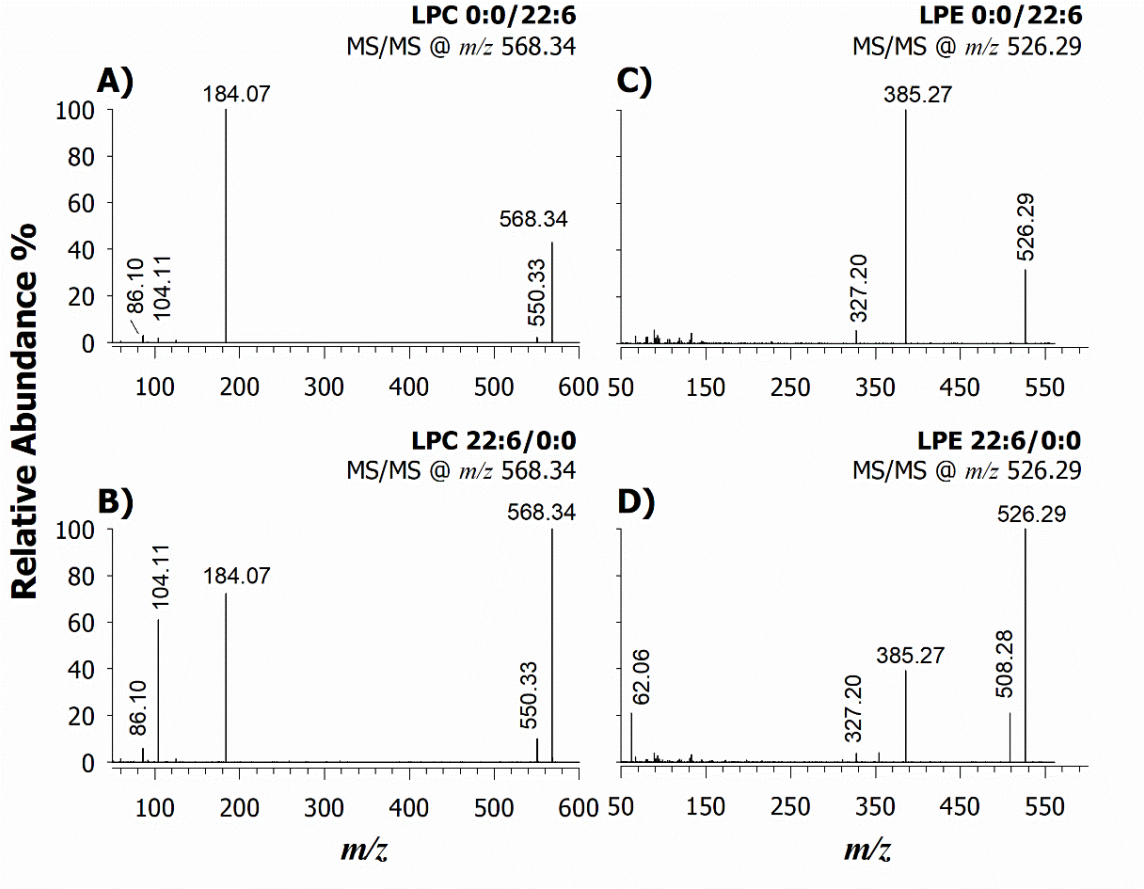

Figure S4. Tandem MS spectra of protonated adducts ($[M+H]^+$) detected at *m/z* 568.34, corresponding to LPC 0:0/22:6 (**A**) and LPC 22:6/0:0 (**B**), and at *m/z* 526.29,corresponding to LPE 0:0/22:6 (**C**) and LPE 22:6/0:0 (**D**). Fragmentations were achieved in the HCD cell of the Q-Exactive spectrometer, using a 20% NCE. Since a resolving power equal to 35000 was adopted, *m/z* values were rounded off to the second decimal place

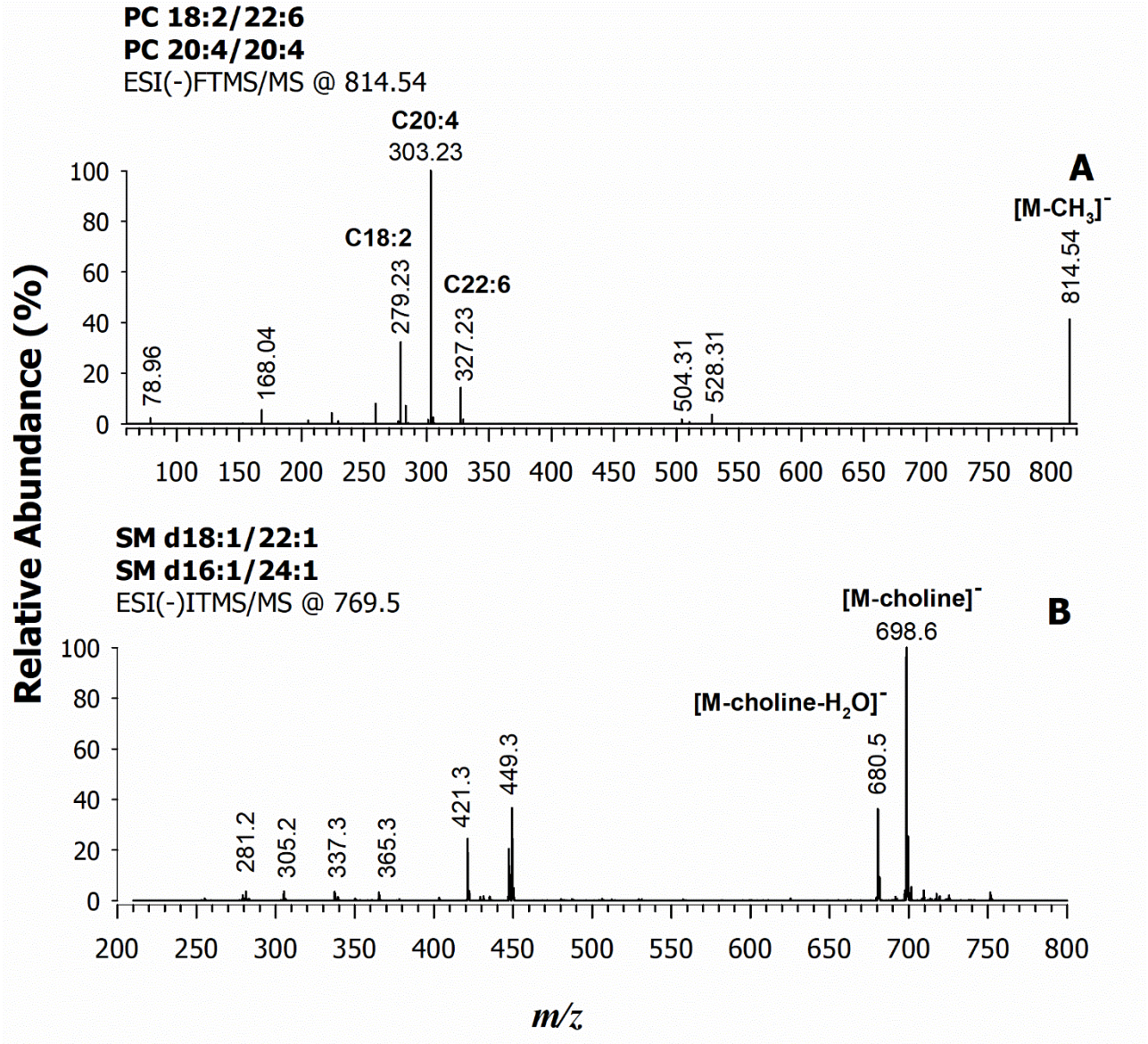

Figure S5. A) ESI(-)-FT-MS/MS spectrum obtained for the demethylated adduct ($[M\text{-}CH_3]^-$) detected at *m/z* 814.5392, corresponding to two isomeric species, PC 18:2/22:6 and PC 20:4/20:4, using a 20% NCE. **B)** ESI(-)-LIT-MS/MS spectrum of the demethylated adduct ($[M\text{-}CH_3]^-$) detected at *m/z* 769.5 corresponding to isomeric SM d18:1/22:1 and d16:1/24:1 species. The last spectrum was registered by using a linear ion trap with collision ion energy fixed at 45%