

Supplementary Data

Table S1. List of identified phosphatidylcholines in salmon tissue in the positive ion mode

[M + Na] ⁺	Phosphatidylcholine	MS/MS scanning		
		Polar head group	Fatty acid 1	Fatty acid 2
782.4	16:0-18:1 PtdCho	NL 183.1 (phosphocholine)	NL 256.0 (16:0)	NL 282.0 (18:1)
802.4	16:0-20:5 PtdCho	NL 183.1 (phosphocholine)	NL 256.0 (16:0)	NL 302.0 (20:5)
802.4	18:2-18:3 PtdCho	NL 183.1 (phosphocholine)	NL 280.0 (18:2)	NL 278.0 (18:3)
804.5	16:0-20:4 PtdCho	NL 183.1 (phosphocholine)	NL 256.0 (16:0)	NL 304.0 (20:4)
808.4	16:0-20:2 PtdCho	NL 183.1 (phosphocholine)	NL 256.0 (16:0)	NL 308.0 (20:2)
828.4	16:0-22:6 PtdCho	NL 183.1 (phosphocholine)	NL 256.0 (16:0)	NL 328.0 (22:6)
850.4	18:3-22:6 PtdCho	NL 183.1 (phosphocholine)	NL 278.0 (18:3)	NL 328.0 (22:6)
852.4	18:2-22:6 PtdCho	NL 183.1 (phosphocholine)	NL 280.0 (18:2)	NL 328.0 (22:6)
852.4	20:3-20:5 PtdCho	NL 183.1 (phosphocholine)	NL 306.0 (20:3)	NL 302.0 (20:5)
854.4	18:1-22:6 PtdCho	NL 183.1 (phosphocholine)	NL 282.0 (18:1)	NL 328.0 (22:6)
874.4	20:5-22:6 PtdCho	NL 183.1 (phosphocholine)	NL 302.0 (20:5)	NL 328.0 (22:6)
878.5	20:5-22:4 PtdCho	NL 183.1 (phosphocholine)	NL 302.0 (20:5)	NL 332.0 (22:4)
880.5	20:2-22:6 PtdCho	NL 183.1 (phosphocholine)	NL 308.0 (20:2)	NL 328.0 (22:6)
882.5	20:2-22:5 PtdCho	NL 183.1 (phosphocholine)	NL 308.0 (20:2)	NL 330.0 (22:5)
882.5	20:3-22:4 PtdCho	NL 183.1 (phosphocholine)	NL 306.0 (20:3)	NL 332.0 (22:4)

Table S2. List of identified PE, PS, and PI in salmon tissue in the negative ion mode using the precursor ion (PI) scanning mode

[M - H]⁻	PE	MSMS scanning		
		Polar head group	Fatty acid 1	Fatty acid 2
736.7	16:0-20:5 PtdEtn	PI 196.0 (glycerol phosphoethanolamine)	PI 255.0 (16:0)	PI 301.0 (20:5)
758.4	18:3-20:5 PtdEtn	PI 196.0	PI 277.0 (18:3)	PI 301.0 (20:5)
760.6	18:2-20:5 PtdEtn	PI 196.0	PI 279.0 (18:2)	PI 301.0 (20:5)
762.6	16:0-22:6 PtdEtn	PI 196.0	PI 255.0 (16:0)	PI 327.0 (22:6)
762.6	18:1-20:5 PtdEtn	PI 196.0	PI 281.0 (18:1)	PI 301.0 (20:5)
762.6	18:2-20:4 PtdEtn	PI 196.0	PI 279.0 (18:2)	PI 303.0 (20:4)
764.0	16:0-22:5 PtdEtn	PI 196.0	PI 255.0 (16:0)	PI 329.0 (22:5)
764.0	18:0-20:5 PtdEtn	PI 196.0	PI 283.0 (18:0)	PI 301.0 (20:5)
764.0	18:1-20:4 PtdEtn	PI 196.0	PI 281.0 (18:1)	PI 303.0 (20:4)
786.6	18:2-22:6 PtdEtn	PI 196.0	PI 279.0 (18:2)	PI 327.0 (22:6)
788.3	18:2-22:5 PtdEtn	PI 196.0	PI 279.0 (18:2)	PI 329.0 (22:5)
790.0	18:0-22:6 PtdEtn	PI 196.0	PI 283.0 (18:0)	PI 327.0 (22:6)
790.0	18:1-22:5 PtdEtn	PI 196.0	PI 281.0 (18:1)	PI 329.0 (22:5)
808.8	20:5-22:6 PtdEtn	PI 196.0	PI 301.0 (20:5)	PI 327.0 (22:6)
812.9	20:3-22:6 PtdEtn	PI 196.0	PI 305.0 (20:3)	PI 327.0 (22:6)
814.8	20:2-22:6 PtdEtn	PI 196.0	PI 307.0 (20:2)	PI 327.0 (22:6)
834.7	22:6-22:6 PtdEtn	PI 196.0	PI 327.0 (22:6)	PI 327.0 (22:6)
836.0	22:5-22:6 PtdEtn	PI 196.0	PI 329.0 (22:5)	PI 327.0 (22:6)
838.6	22:4-22:6 PtdEtn	PI 196.0	PI 331.0 (22:4)	PI 327.0 (22:6)
[M - H]⁻ PS				
806.1	16:0-22:6 PtdSer	PI 153.0 (glycerol phosphate derivative)	PI 255.0 (16:0)	PI 327.0 (22:6)
808.1	18:0-20:5 PtdSer	PI 153.0	PI 283.0 (18:0)	PI 301.0 (20:5)
834.1	18:0-22:6 PtdSer	PI 153.0	PI 283.0 (18:0)	PI 327.0 (22:6)
836.4	18:0-22:5 PtdSer	PI 153.0	PI 283.0 (18:0)	PI 329.0 (22:5)
880.0	22:5-22:6 PtdSer	PI 153.0	PI 329.0 (22:5)	PI 327.0 (22:6)
[M - H]⁻ PI				
883.1	16:0-22:5 PtdIns	PI 241.0 (cyclic inositol phosphate)	PI 255.0 (16:0)	PI 329.0 (22:5)
883.1	18:0-20:5 PtdIns	PI 241.0	PI 283.0 (18:0)	PI 301.0 (20:5)
909.8	18:0-22:6 PtdIns	PI 241.0	PI 283.0 (18:0)	PI 327.0 (22:6)
909.8	20:1-20:5 PtdIns	PI 241.0	PI 309.0 (20:1)	PI 301.0 (20:5)

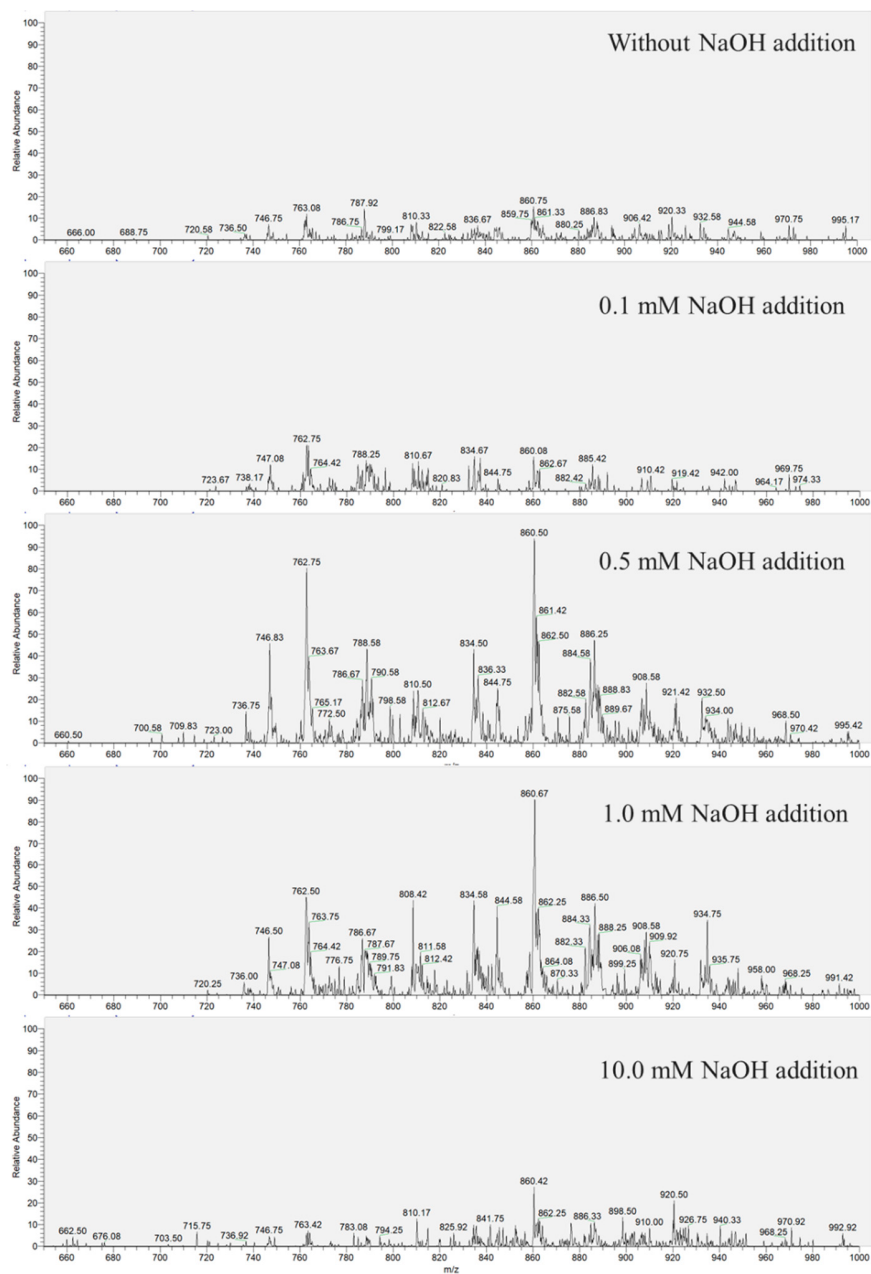


Figure S1. Precursor ion (PI) scanning (196.0) of a salmon extract at different concentrations of sodium hydroxide addition in order to optimize the ionization of phospholipids in the negative mode.