

Fig. S2. The fatty acid compositions of PCs are obtained by full fragmentation. The negative ion modes were used for LC/MS/MS data acquisition. The VLC-PUFA-containing PCs are depicted; (A) PC54:12 (m/z 1076 (M+CH3COO⁻) corresponds to m/z 1018 (M+H⁺) in positive mode) is composed of FA32:6 (m/z 467) and FA22:6 (m/z 327). (B) PC56:12 (m/z 1104 (M+CH3COO⁻) corresponds to m/z 1046 (M +H⁺) in positive mode) is composed of FA34:6 (m/z 495) and FA22:6 (m/z 327). (C) PC58:12 (m/z 1132 (M+CH3COO⁻) corresponds to m/z 1074 (M+H⁺) in positive mode) is composed of FA36:6 (m/z 523) and FA22:6 (m/z 327). DHA-containing PCs are on the second row; (D) PC38:6 (m/z 864 (M+CH3COO⁻) corresponds to m/z 806 (M+H+) in positive mode) is composed of FA16:0 (m/z 255) and FA22:6 (m/z 327). (E) PC40:6 (m/z 892 (M+CH3COO⁻) corresponds to m/z 834 (M+H⁺) in positive mode) is composed of FA18:0 (m/z 283) and FA22:6 (m/z 327.0). (F) PC44:12 (m/z 936 (M+CH3COO-) corresponds to m/z 878 (M+H+) in positive mode) is composed of two FA22:6s (m/z 327.0). AA-containing PCs are at the third row; (G) PC36:4 (m/z 840 (M+CH3COO⁻) corresponds to m/z 782 (M+H⁺) in positive mode) is composed of FA16:0 (m/z 255) and FA20:4 (m/z 303). (H) PC38:4 (m/z 868 (M+CH3COO-) corresponds to m/z 810 (M+H+) in positive mode) is composed of FA18:0 (m/z 283) and FA20:4 (m/z 303). (/) PC38:5 (m/z 866 (M+CH3COO⁻) corresponds to m/z 808 (M+H⁺) in positive mode) is composed of FA18:1 (m/z 281) and FA20:4 (m/z 303). This peak is also possible from PC38:6 isotopes (two carbons being naturally C13 labeled). That will produce FA16:0 (m/z 255) and FA22:6(m/z 329 when two carbons are C13), or FA16:0 (m/z 256 when one carbon is C13) and FA22:6 (m/z 328 when one carbon is C13).