

## Concentration and Composition of Odd-Chain Fatty Acids in Phospholipids and Triacylglycerols in Chinese Human Milk throughout Lactation

Xiao-Yan Chen, et al

**Supplemental Table 1** Correlations of PL-OCFA and TAG-OCFA with food groups intake (energy-adjusted)

	PL-OCFA	TAG-OCFA
Dairy products	0.031	0.004
Vegetables	0.056	-0.152*
Fruits	0.187***	-0.233***
Cereals	-0.214***	0.023
Meat	0.009	-0.028

Values were expressed as correlation coefficient and Pearson's Correlation was performed to analyze the correlation of PL-OCFA and TAG-OCFA with food groups intake, adjusted for total daily energy intake. \* indicated  $p < 0.05$ ; \*\*\* indicated  $p < 0.001$ . Abbreviation: PL-OCFA, odd chain fatty acid-containing phospholipids; TAG-OCFA, odd chain fatty acid-containing triacylglycerols.

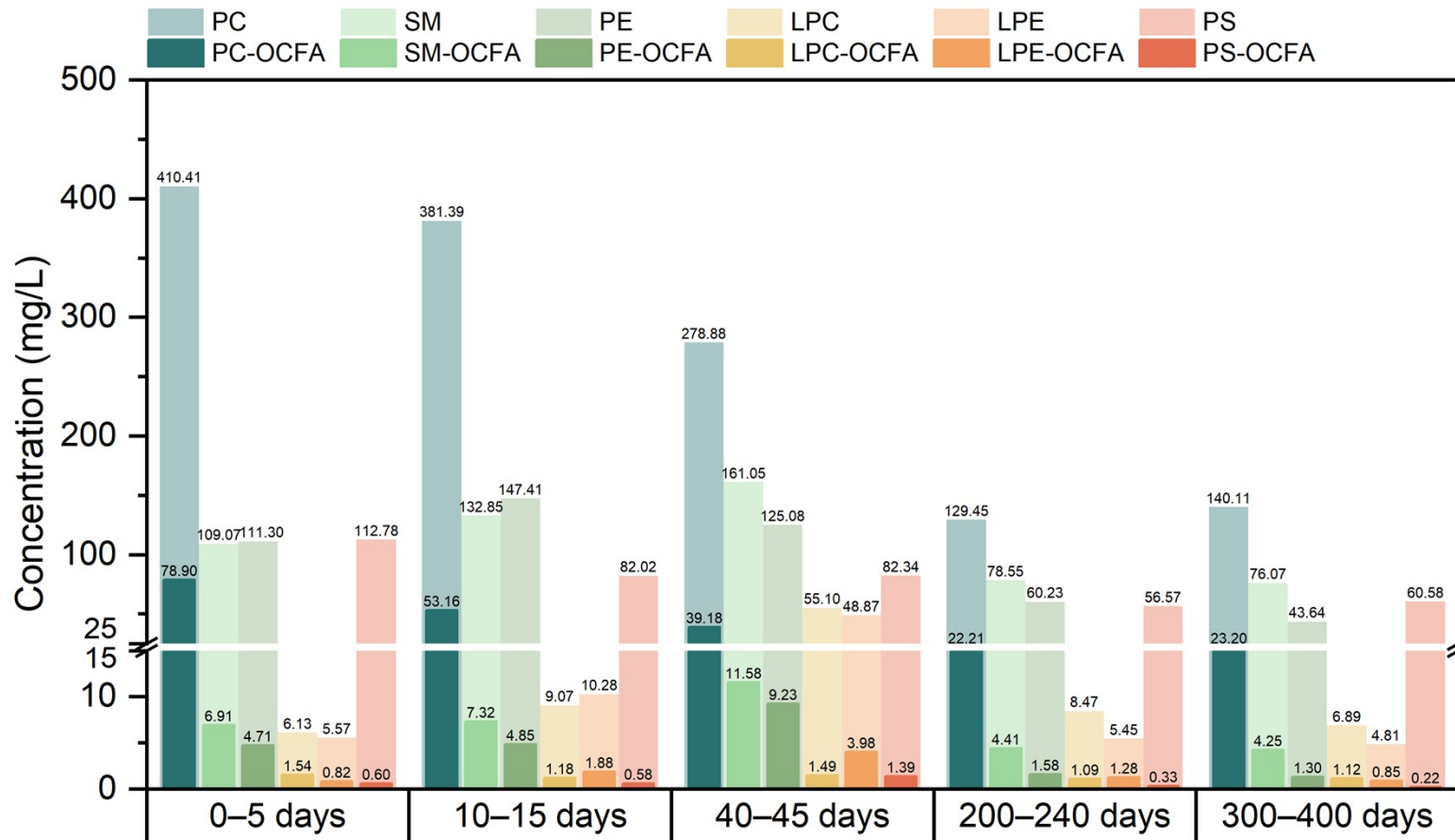
**Supplemental Table 2** List of OCFA-containing phospholipid identified in human milk

Molecular species	Fatty acyl group ( <i>sn1/sn2</i> )	m/z in MS/MS (precursor ion>product ion)
PE(33:1)	15:0/18:1	704.50>563.50
PE(P-35:2)	P-17:0/18:2	714.55>573.55
PE(P-35:1)	P-17:0/18:1	716.55>575.55
PE(35:1)	17:0/18:1	732.55>591.55
PE(37:3)	19:0/18:3	756.55>615.55
PE(37:2)	19:0/18:2	758.55>617.55
PE(37:1)	19:0/18:1	760.60>619.60
PE(39:5)	19:0/20:5	780.55>639.55
PE(39:4)	19:0/20:4	782.55>641.55
PE(39:3)	19:0/20:3	784.60>643.60
PC(29:0)	14:0/15:0	692.50>184.10
PC(31:1)	13:0/18:1	718.55>184.10
PC(31:0)	13:0/18:0	720.55>184.10
PC(33:2)	15:0/18:2	744.55>184.10
PC(33:1)	15:0/18:1	746.55>184.10
PC(33:0)	15:0/18:0	748.60>184.10
PC(P-35:2)	P-17:0/18:2	756.60>184.10
PC(P-35:1)	P-17:0/18:1	758.60>184.10
PC(35:2)	17:0/18:2	772.60>184.10
PC(35:1)	17:0/18:1	774.60>184.10
PC(37:3)	19:0/18:3	798.60>184.10
PC(37:2)	19:0/18:2	800.60>184.10
PC(37:1)	19:0/18:1	802.65>184.10
PC(39:5)	19:0/20:5	822.60>184.10

PC(39:4)	19:0/20:4	824.60>184.10
PC(39:3)	19:0/20:3	826.65>184.10
LPE(17:0)	17:0	468.30>327.30
LPE(19:0)	19:0	496.35>355.35
LPE(P-17:0)	P-17:0	452.30>311.30
LPE(P-19:0)	P-19:0	480.35>339.35
PS(33:1)	15:0/18:1	748.50>563.50
PS(35:2)	17:0/18:2	774.55>589.50
PS(37:3)	19:0/18:3	800.55>615.55
PS(37:2)	19:0/18:2	802.55>617.55
PS(39:5)	19:0/20:5	824.55>639.55
PS(39:4)	19:0/20:4	826.55>641.55
PS(39:3)	19:0/20:3	828.60>643.55
SM(d33:1)	d18:1/15:0	689.55>184.10
SM(d35:1)	d18:1/17:0	717.60>184.10
SM(d37:1)	d18:0/19:0	745.60>184.10
SM(d39:2)	d18:2/21:0	771.65>184.10
SM(t38:2)	d18:1/21:0	773.60>184.10
SM(d39:0)	d18:0/21:0	775.65>184.10
SM(d41:2)	d18:2/23:0	799.65>184.10
SM(d41:1)	d18:1/23:0	801.70>184.10
SM(d41:0)	d18:0/23:0	803.70>184.10
LPC(P-17:0)	P-17:0	494.35>184.10
LPC(P-19:0)	P-19:0	522.40>184.10

**Supplemental Table 3** List of OCFAs-containing phospholipid identified in human milk

TAG	Composition	[M+NH <sub>4</sub> ] <sup>+</sup>	[M+H-FA] <sup>+</sup>
O-Ha-P	C18:1/C17:0/C16:0	864.8044	577.5158
O-O-Pa	C18:1/C18:1/C15:0	862.7899	603.5872
O-L-Pa	C18:1/C18:2/C15:0	860.7766	601.5839
L-He-P	C18:2/C17:1/C16:0	860.7766	575.5540
He-He-He	C17:1/C17:1/C17:1	860.7766	575.5540
O-O-Ha	C18:1/C18:1/C17:0	890.8212	603.5801
O-L-Ha	C18:1/C18:2/C17:0	888.8063	601.5718
O-Ln-Ha	C18:1/C18:3/C17:0	886.7872	599.5709



**Supplemental Figure 1** The concentration of sub-class PLs and PL-OCFA across lactation periods. Values were expressed as mean. Abbreviation: PL-OCFA, odd chain fatty acid-containing phospholipids; PLs, phospholipids; PC-OCFA, odd chain fatty acid-containing phosphatidylcholines;

PC, phosphatidylcholines; SM-OCFA, odd chain fatty acid-containing sphingomyelins; SM, sphingomyelins; PE-OCFA, odd chain fatty acid-containing phosphatidylethanolamines; PE, phosphatidylethanolamines; LPC-OCFA, odd chain fatty acid-containing lysophosphatidylcholines; LPC, lysophosphatidylcholines; LPE-OCFA, odd chain fatty acid-containing lysophosphatidylethanolamines; LPE, lysophosphatidylethanolamines; PS-OCFA, odd chain fatty acid-containing phosphatidylserines; PS, phosphatidylserines.