



Fatty acid and triacylglycerol comparison of infant formulas on the Chinese market

Yujie Chen^{a, c}, Xin Zhang^{b, c}, Donggang Li^{b, c}, Huaxi Yi^{a, c}, Tao Xu^{a, c}, Siming Li^{a, c}, Lanwei Zhang^{a, b, c, *}

^a College of Food Science and Engineering, Ocean University of China, Qingdao, China

^b The Academy of Quality Supervision and Inspection in Heilongjiang Province, Harbin, China

^c Biotechnology Centre of Gansu Haling, Lanzhou, China

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ABSTRACT

Fatty acid (FA) and triacylglycerol (TAG) composition plays an important role in the nutritional value of infant formulas. The profiles of FAs and TAGs, and regioisomers (rac) of dioleoyl-palmitoylglycerol (OPO) and dipalmitoyl-oleoylglycerol (PPO) in ten brands of infant formulas were analysed and compared between infant formulas labelled as containing rac-OPO (OPO-Fs) or not labelled as such (OPO-NFs). The predominant difference was that OPO-Fs mainly contained rac-OPO (~70%) and rac-PPO (>95%), while OPO-NFs mainly contained rac-OOP (65.24–100%) and rac-POP (~90%). With rac-OPO supplementation, the levels of saturated FAs (especially palmitic acid) and TAGs improved. The same results were observed in infant formulas supplemented with palm searin. The levels of short chain FAs, odd-numbered saturated FAs, stearic, myristoleic and palmitoleic acids were mainly affected by the basic materials of infant formulas. Coconut and palm kernel oil addition enhanced the concentrations of medium chain FAs and TAGs.

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1. Introduction

Human milk is recommended as the best choice for providing the nutritional necessities for newborns, particularly during the first 6 months of life. However, breastfeeding is sometimes not possible for many reasons, such as health problems and medication, as well as social or cultural reasons (Barreiro, Regal, López-Racamonge, Cepeda, & Fente, 2017; Tu, Ma, Bai, & Du, 2017). In these circumstances, commercial infant formulas based on mammalian milk are considered as the best substitutes for human milk.

The composition and nutrition of infant formulas should be designed to mimic human milk, which supplies complete nutrition for infants, as closely as possible. Lipids are the chief nutritional ingredients for fulfilling a newborn's needs, providing almost 50% of the total energy and essential fatty acids (FAs) for infants (Bourlieu et al., 2015). Different infant formula brands have different ingredients, resulting in big differences in fat chemical composition. The profiles of FAs and triacylglycerols (TAGs) can have an enormous influence on the physical properties and

physiological function of fat. Therefore, the profiles and differences in FAs and TAGs in the different brands of infant formulas need to be made clear.

FA profiles of infant formulas are the one of the most basic aspects in simulating human milk. There are many standards about FA supplementation in infant formulas, such as the relative concentrations of docosahexaenoic acid (DHA) and arachidonic acid (ARA), the levels of the sum of lauric and myristic acids and the ratio of linoleic/ α -linolenic acids (LA/ALA) (Berthold et al., 2005). Polyunsaturated FAs (PUFAs), especially DHA and ARA, have numerous positive developmental outcomes for infants including cognitive function, visual function and immune function and infection, are prerequisite additions into infant formulas (Lien, Richard, & Hoffman, 2018).

TAGs present >98% of lipids in infant formulas and human milk, the structure of which plays an important role in lipids digestion and absorption in infants. Long chain saturated FAs (LCFAs), especially palmitic acid (PA), are mainly located at the TAG sn-2 position in human milk. The specific distribution of PA in human milk results in significant reduction of extraction of faecal soap FAs and calcium malabsorption and promoting early bone mineralisation (Bar-Yoseph, Lifshitz, & Cohen, 2013; Bar-Yoseph, Lifshitz, Cohen,

* Corresponding author. Tel.: +86 451 86282901.

E-mail address: zhanglw@hit.edu.cn (L. Zhang).

Malard, & Xu, 2016; Innis & Nelson, 2013; Wan et al., 2016). In human milk dioleoyl-palmitoylglycerol (OPO) and oleoyl-palmitoyl-linoleoylglycerol (OPL) are the two most abundant TAGs, the main regioisomers of which are 1,3-dioleoyl-2-palmitoylglycerol (rac-OPO) and 1-oleoyl-2-palmitoyl-3-linoleoylglycerol (rac-OPL), respectively (Kallio, Nylund, Bostrom, & Yang, 2017). To mimic human milk, much attention has been paid to supplement rac-OPO in infant formulas. rac-OPO is allowed as a nutrient fortifier supplement in commercial infant formulas in China, which results in a high price for the formulas compared with those that are not labelled as rac-OPO formulas. However, the differences in composition of FAs and TAGs in different ingredients lists for infant formulas are not totally clear.

The composition of FAs and TAGs have been paid much attention in recent years. The composition of FAs, sn-2 FAs and TAGs were analysed in plant-oil formula, cows' milk formula and goats' milk formula (Sun et al., 2016, 2018b; Sun, Wei, Su, Zou, & Wang, 2018a). The FA composition in Spanish market infant formulas were also analysed and compared with human milk (Barreiro et al., 2017), as was the TAG composition of imported infant formulas in the Chinese market (Tu et al., 2017). However, there was no attention paid to the differences between infant formulas labelled as containing rac-OPO (OPO-Fs) and those not so labelled (OPO-NFs).

The purpose of our study was to compare the FA and TAG composition of OPO-Fs and OPO-NFs in the Chinese market. The regioisomers of OPO and PPO were also analysed and compared in OPO-Fs and OPO-NFs. The differences from other fat source such as milk fat, palm kernel oil and coconut oil, and common plant oil (rapeseed, sunflower, soybean, corn oil) were also compared.

2. Materials and methods

2.1. Infant formula samples

Ten brands of infant formula in the Chinese market were collected, including five brand formulas labelled as containing rac-OPO (OPO-F1–5), and five brand formulas not labelled as containing rac-OPO (OPO-NF1–5). The basic materials of OPO-F1–4 were whole milk, while OPO-F5 and OPO-NF1–5 were skimmed milk. The infant formulas of OPO-F1,3–5 and OPO-NF1–4 were supplemented with coconut or palm kernel oil. According to ingredient lists, the supplementation of other plant oils was as follows: sunflower oil was added into OPO-F1,3–5 and OPO-NF1–4; OPO-NF5 was supplemented with high oleic sunflower oil; rapeseed oil was supplemented into OPO-F1,3–5 and OPO-NF2–5; OPO-F2,5 and OPO-NF1,5 were supplemented with soybean oil; OPO-NF4–5 were supplemented with corn oil; palm oil was supplemented into OPO-NF1–2. All samples were on the first-stage infant formulas (0–6 months), and had DHA and ARA labels.

2.2. Reagents and standards samples

The racemic dipalmitoyl-oleoylglycerol (rac-PPO, rac-POP) and dioleoyl-palmitoylglycerol (rac-OPO, rac-OOP) standards were purchased from Larodan Fine Chemicals (Malmö, Sweden). The standard mixture of FAMES was purchased from Sigma Aldrich Chemical Co. Ltd. (Shanghai, China). All solvents were HPLC or HPLC-MS grade and purchased from Merck (Darmstadt, Germany).

2.3. Fat extraction from the infant formulas

Fat fraction from the infant formulas were extracted using the Folch procedure (Folch, Lee, & Sloane-Stanley, 1957). Briefly, 1 g formula powder was dissolved in 10 mL water (45 °C). Then 40 mL chloroform:methanol (2:1, v/v) were added and mixed thoroughly,

then cooled in an ice bath for 30 min and then centrifuged. The chloroform layers were collected and the water layers were re-extracted twice with chloroform:methanol (2:1, v/v, 20 mL each time). The organic phases were evaporated using a rotary vacuum evaporator. The total lipids obtained were stored at –20 °C for further analysis.

2.4. Fatty acid analysis

Fatty acid methyl esters (FAMES) were prepared as follows: in brief, 20 mg fat were first reacted with 0.5 M NaOH–MeOH, at 100 °C for 5 min. Then the mixture was reacted with 14% BF₃ at 100 °C for 30 min. FAMES were extracted with 200 µL hexane, and subsequently analysed on a gas chromatograph (GC) (Thermo-Fisher Scientific, Waltham, MA, USA) equipped with a flame ionisation detector, and a capillary column (Supelco SP 2560, 100 m × 0.25 mm × 0.2 µm, Sigma–Aldrich, St. Louis, MO, USA). The oven temperature was maintained at 100 °C for 5 min, then increased at 4 °C min⁻¹ to 240 °C, and finally maintained at 240 °C for 25 min. The temperature of the injector and detector was 260 °C. Helium was the carrier gas, at a flow rate of 0.8 mL min⁻¹.

2.5. TAG analysis

The identification of TAGs was using a Bruker maXis UHR-TOF-MS (Bruker, Daltonics, Bremen, Germany) combined with a Zorbax Eclipse Plus C18 column (1.8 µm, 2.1 × 100 mm Agilent Technologies, Wilmington, DE, USA). The mobile phase gradient was as follows: 0–5 min 90% A + 10% B; 5–25 min 90–60% A + 10–40% B; 25–60 min 60–40% A + 40–60% B; 60–66 min 40% A + 60% B; where A was a mixture of acetonitrile-methanol-water (19:19:2, by vol) with 10 mM ammonium acetate and 0.1% formic acid, B was 2-propanol with 10 mM ammonium acetate and 0.1% formic acid. The flow rate was 0.2 mL min⁻¹, injection volume was 2 µL, column temperature was 45 °C, and sample concentration was 0.5 mg mL⁻¹.

The parameters of Q-TOF mass spectrometer were as follows: data acquisition proceeded in positive ion electrospray ionisation (ESI) mode; source gas flow, 6 L min⁻¹; source temperature, 180 °C; mass range *m/z*, 50–1200.

2.6. Analysis of regioisomers of OPO and PPO

In this study, off-line compressive 2D LC was used for analysis of the regioisomers of OPO and PPO. TAG regioisomer analysis was performed on a liquid chromatograph Agilent 1290 Series (Agilent Technology, Waldbronn, Germany), equipped with an evaporative light-scattering detector (ELSD). The ELSD was set at 40 °C at a gas pressure of 30 psi and a gain of 150. The mobile phase and column conditions for the first step were the same as for TAG species analysis. The fractions corresponding to OPO and PPO were collected, then concentrated by nitrogen and redissolved with hexane. A Varian ChromSpher 5 Lipids column (5 µm, 250 mm × 4.6 mm, Agilent Technologies, Wilmington, DE, USA) was used as the second step to separate the regioisomers of OPO and PPO. Column conditions were as follows: flow rate, 0.5 mL min⁻¹; injection volume of 5 µL, column temperature of 30 °C, and the mobile phase gradient: 0 min 98% A + 2% B; 10 min 92% A + 8% B; 10–40 min 92% A + 8% B, where A was dichloromethane, B was acetone. The chromatographic system was equilibrated between injections for at least 30 min.

2.7. Statistical analysis

All analyses were of triplicate formula samples; results were expressed as means ± standard deviations (SD). The data were

subjected to one-way analysis of variance (ANOVA) and Turkey's test using the Statistical Package for the Social Sciences (Version 20.0, SPSS Inc., Chicago, USA). Results were considered statistically significant at $p < 0.05$. The PCA analysis were done using SIMCA-P software (Version 14.1, Demo Umetrics, Umea, Sweden).

3. Results and discussion

3.1. Fatty acid profiles in the infant formulas

FA and TAG compositions play an important role in the nutritional value of infant formulas; the different fat source supplementations resulted in a lot of differences in FA and TAG compositions. FA profiles of the infant formulas are presented in Tables 1 and 2. Thirty FAs were identified and classified into saturated, monounsaturated and polyunsaturated FAs (SFAs, MUFAs and PUFAs, respectively). To obtain more visualised information on the FAs in the different infant formulas, PCA analysis was applied. The PCA score scatter plot showed that the samples from OPO-F1–4 clustered relatively close together and were distributed on the positive side of PC1. OPO-F5 and OPO-NF1–5 were negatively scored on PC1. With regard to PC2, OPO-F1,3–5 and OPO-NF1–4 were relatively close together, while OPO-F2 and OPO-NF5 appeared on the negative side (Fig. 1A).

SFAs, which approximately account for 40% of total FAs in human milk (Barreiro, Diaz-Bao, Cepeda, Regal, & Fente, 2018), ranged

from 33.75% to 47.88% and 22.04%–39.24% in OPO-Fs and OPO-NFs, respectively. Therefore, compared with OPO-NFs, the contents of SFAs in OPO-Fs were more similar to those in human milk. SFAs were classified as short-chain FAs (SCFAs, C4–C6), medium-chain FAs (MCFAs, C8–C14), and long-chain FAs (LCFAs, C15–C24).

The loading plot of PCA showed that SCFAs were associated with the OPO-F1–4 group, the basic materials of which were whole milk (Fig. 1B). The contents of SCFAs in OPO-F1–4 (1.07–1.46%) were significantly higher than those in OPO-F5 and OPO-NF1–5 (0.14–0.70%), the basic materials were skimmed milk ($p < 0.001$, Tables 1 and 2). Milk fat was the only source of SCFAs in infant formulas; they were not detected in plant oil and may be considered as markers of milk fat (Sun et al., 2016). In human milk SCFAs are rarely detected (Zou et al., 2013).

MCFAs are commonly supplemented into infant formulas, particularly for premature infants, because they can be directly absorbed by the portal vein and rapidly generate energy for infants (Billeaud et al., 2018). Coconut oil and palm kernel oil, which contained high concentrations of MCFAs, especially lauric acid (C12:0) and myristic acid (C14:0), are usually used to supplement MCFAs in infant formulas (Chai et al., 2018; Lee et al., 2018; Ponphaiboon, Limmatvapirat, Chaidedgumjorn, & Limmatvapirat, 2018). In the PC2 vector of the PCA, the group of OPO-F1,3–5 and OPO-NF1–4 were mainly linked to MCFAs (Fig. 1A and B). The results in Tables 1 and 2 show that the values of MCFAs in infant formulas that were supplemented with coconut or palm kernel oil (OPO-F1,3–5 and

Table 1
Fatty acid profiles of infant formulas in OPO-Fs.^a

Fatty acid	OPO-F1	OPO-F2	OPO-F3	OPO-F4	OPO-F5
C4:0	0.57 ^c ± 0.04	0.79 ^a ± 0.05	0.6 ^c ± 0.02	0.65 ^b ± 0.02	0.03 ^d ± 0.00
C6:0	0.50 ^a ± 0.01	0.67 ^c ± 0.01	0.49 ^a ± 0.00	0.53 ^b ± 0.00	0.11 ^d ± 0.00
C8:0	0.88 ^a ± 0.01	0.47 ^b ± 0.00	0.59 ^c ± 0.00	0.71 ^d ± 0.00	1.20 ^e ± 0.01
C10:0	1.28 ^a ± 0.00	1.14 ^b ± 0.00	0.97 ^c ± 0.00	1.07 ^d ± 0.00	0.98 ^c ± 0.00
C11:0	0.06 ^a ± 0.00	0.03 ^b ± 0.00	0.06 ^a ± 0.00	0.07 ^a ± 0.00	ND
C12:0	7.78 ^a ± 0.01	1.69 ^b ± 0.01	2.68 ^c ± 0.01	3.60 ^d ± 0.01	7.70 ^e ± 0.01
C13:0	0.06 ^a ± 0.00	0.09 ^b ± 0.00	0.05 ^c ± 0.00	0.05 ^c ± 0.00	ND
C14:0	5.41 ^a ± 0.00	4.67 ^b ± 0.00	3.87 ^c ± 0.01	4.30 ^d ± 0.00	3.43 ^e ± 0.00
C14:1	0.21 ^a ± 0.00	0.35 ^b ± 0.0	0.21 ^a ± 0.00	0.22 ^a ± 0.00	ND
C15:0	0.29 ^a ± 0.00	0.48 ^b ± 0.00	0.30 ^c ± 0.00	0.31 ^c ± 0.00	0.05 ^d ± 0.00
C16:0	22.24 ^a ± 0.03	29.08 ^b ± 0.02	24.35 ^c ± 0.01	24.71 ^d ± 0.05	19.47 ^e ± 0.01
C16:1	0.44 ^a ± 0.00	0.59 ^b ± 0.00	0.39 ^c ± 0.00	0.46 ^d ± 0.00	0.14 ^e ± 0.00
C17:0	0.21 ^a ± 0.00	0.29 ^b ± 0.02	0.22 ^{ac} ± 0.01	0.23 ^c ± 0.01	0.09 ^d ± 0.00
C18:0	5.94 ^a ± 0.00	7.85 ^b ± 0.00	6.60 ^c ± 0.01	6.68 ^d ± 0.01	3.72 ^e ± 0.00
C18:1n9	35.02 ^a ± 0.03	28.85 ^b ± 0.06	37.24 ^c ± 0.01	36.45 ^d ± 0.00	41.85 ^e ± 0.02
C18:2n6	15.50 ^a ± 0.02	18.56 ^b ± 0.02	17.43 ^c ± 0.02	16.30 ^d ± 0.02	16.66 ^e ± 0.04
C20:0	0.31 ^a ± 0.00	0.30 ^a ± 0.00	0.31 ^a ± 0.00	0.31 ^a ± 0.00	0.26 ^b ± 0.00
C18:3n6	0.03 ± 0.01	0.04 ± 0.04	0.03 ± 0.01	0.05 ± 0.04	0.05 ± 0.05
C20:1	0.35 ^a ± 0.00	0.22 ^b ± 0.00	0.33 ^c ± 0.00	0.40 ^d ± 0.00	0.29 ^e ± 0.00
C18:3n3	1.66 ^a ± 0.01	2.84 ^b ± 0.01	1.93 ^c ± 0.00	1.63 ^d ± 0.01	2.12 ^e ± 0.01
C20:2	0.05 ^a ± 0.00	0.04 ^b ± 0.00	0.05 ^a ± 0.00	0.05 ^a ± 0.00	0.06 ^a ± 0.01
C22:0	0.24 ^a ± 0.00	0.19 ^b ± 0.01	0.27 ^c ± 0.00	0.26 ^c ± 0.00	0.40 ^d ± 0.00
C20:3n6	0.06 ^a ± 0.00	0.04 ^b ± 0.00	0.06 ^a ± 0.01	0.06 ^a ± 0.00	0.05 ^c ± 0.00
C22:1n9	0.05 ^a ± 0.00	ND	0.01 ^b ± 0.01	0.08 ^c ± 0.00	ND
C20:4n6	0.44 ^a ± 0.00	0.26 ^b ± 0.01	0.42 ^c ± 0.01	0.41 ^c ± 0.00	0.54 ^d ± 0.01
C23:0	0.04 ± 0.01	0.04 ± 0.00	0.04 ± 0.01	0.05 ± 0.01	0.04 ± 0.00
C24:0	0.12 ^a ± 0.00	0.10 ^b ± 0.00	0.12 ^a ± 0.00	0.12 ^a ± 0.00	0.27 ^c ± 0.00
C20:5n3	ND	0.10 ^a ± 0.08	0.11 ^a ± 0.01	0.08 ^b ± 0.07	0.11 ^a ± 0.09
C24:1	0.04 ± 0.01	0.01 ± 0.01	0.03 ± 0.01	0.04 ± 0.01	0.03 ± 0.01
C22:6n3	0.19 ^a ± 0.00	0.23 ^b ± 0.01	0.23 ^b ± 0.01	0.17 ^c ± 0.00	0.33 ^d ± 0.00
SFAs	45.93 ± 0.11	47.88 ± 0.12	41.53 ± 0.08	43.65 ± 0.11	37.77 ± 0.04
SCFAs	1.07 ^a ± 0.05	1.46 ^b ± 0.06	1.09 ^a ± 0.02	1.18 ^c ± 0.02	0.14 ± 0.01
MCFAs	15.44 ^a ± 0.02	8.09 ^b ± 0.01	8.20 ^c ± 0.01	9.76 ^d ± 0.01	13.31 ^e ± 0.03
LCFAs	34.80 ^a ± 0.04	43.00 ^b ± 0.05	36.09 ^c ± 0.05	36.97 ^d ± 0.08	27.73 ^e ± 0.01
ONSFAs	0.67 ^a ± 0.10	0.93 ^b ± 0.20	0.67 ^a ± 0.21	0.69 ^a ± 0.16	0.20 ^c ± 0.04
MUFAs	36.11 ^a ± 0.04	30.02 ^b ± 0.07	38.21 ^c ± 0.03	37.65 ^d ± 0.01	42.31 ^e ± 0.04
PUFAs	17.93 ^a ± 0.04	22.11 ^b ± 0.17	20.26 ^c ± 0.07	18.75 ^d ± 0.14	19.92 ^e ± 0.21
LA/ALA	9.35 ^a ± 0.26	6.53 ^b ± 0.09	9.02 ^c ± 0.11	10.01 ^d ± 0.25	7.86 ^e ± 0.03

^a Abbreviations are: SFAs, saturated fatty acids; SCFAs, short-chain SFAs; MCFAs, medium-chain SFAs; LCFAs, long-chain SFAs; ONSFAs, odd-chain number SFAs; MUFAs, monounsaturated fatty acids; PUFAs, polyunsaturated fatty acids; LA/ALA, linoleic acid/ α -linolenic acid. Values are means ± standard deviation (ND, not detected); different superscript letters indicate significant differences ($P < 0.05$) within a row.

Table 2
Fatty acid profiles of infant formulas in OPO-NFs.^a

Fatty acids	OPO-NF1	OPO-NF2	OPO-NF3	OPO-NF4	OPO-NF5
C4:0	0.03 ^a ± 0.00	0.04 ^a ± 0.00	0.03 ^a ± 0.00	0.03 ^a ± 0.01	0.39 ^b ± 0.01
C6:0	0.12 ^a ± 0.00	0.13 ^b ± 0.00	0.14 ^b ± 0.00	0.12 ^a ± 0.00	0.31 ^c ± 0.00
C8:0	1.25 ^a ± 0.01	1.37 ^b ± 0.00	1.46 ^c ± 0.00	1.32 ^d ± 0.00	0.22 ^e ± 0.00
C10:0	1.06 ^a ± 0.01	1.14 ^b ± 0.01	1.20 ^c ± 0.00	1.10 ^d ± 0.00	0.51 ^e ± 0.00
C11:0	ND	ND	ND	ND	0.03 ± 0.01
C12:0	8.41 ^a ± 0.02	8.68 ^b ± 0.01	9.49 ^c ± 0.01	8.23 ^d ± 0.01	0.78 ^e ± 0.00
C13:0	ND	ND	ND	ND	0.03 ± 0.00
C14:0	3.95 ^a ± 0.01	4.02 ^b ± 0.01	4.20 ^c ± 0.01	3.33 ^d ± 0.00	1.96 ^e ± 0.00
C14:1	0.01 ^a ± 0.01	ND	ND	ND	0.11 ^b ± 0.00
C15:0	0.05 ^a ± 0.00	0.05 ^a ± 0.00	0.05 ^a ± 0.00	0.03 ^b ± 0.00	0.21 ^c ± 0.00
C16:0	22.13 ^a ± 0.01	18.30 ^b ± 0.01	8.77 ^c ± 0.02	7.65 ^d ± 0.01	11.29 ^e ± 0.03
C16:1	0.15 ^a ± 0.00	0.13 ^b ± 0.00	0.19 ^c ± 0.00	0.13 ^b ± 0.00	0.39 ^d ± 0.00
C17:0	0.09 ^a ± 0.00	0.09 ^a ± 0.00	0.07 ^b ± 0.00	0.05 ^c ± 0.00	0.19 ^d ± 0.00
C18:0	4.37 ^a ± 0.00	4.46 ^b ± 0.00	3.37 ^c ± 0.00	2.69 ^d ± 0.00	4.88 ^e ± 0.00
C18:1n9c	36.38 ^a ± 0.02	39.24 ^b ± 0.03	48.79 ^c ± 0.1	51.57 ^d ± 0.06	51.62 ^e ± 0.06
C18:2n6c	18.15 ^a ± 0.02	17.93 ^b ± 0.03	17.38 ^c ± 0.03	20.00 ^d ± 0.03	22.27 ^e ± 0.08
C20:0	0.31 ^a ± 0.00	0.31 ^a ± 0.00	0.33 ^{ab} ± 0.00	0.35 ^b ± 0.00	0.31 ^a ± 0.00
C18:3n6	0.07 ± 0.07	0.05 ± 0.05	0.03 ± 0.02	0.02 ± 0.01	0.02 ± 0.01
C20:1	0.32 ^a ± 0.00	0.27 ^b ± 0.00	0.46 ^c ± 0.00	0.42 ^d ± 0.00	0.23 ^e ± 0.00
C18:3n3	1.51 ^a ± 0.00	2.28 ^b ± 0.01	2.17 ^c ± 0.00	1.90 ^d ± 0.01	2.51 ^e ± 0.01
C20:2	0.05 ± 0.00	0.05 ± 0.01	0.06 ± 0.00	0.06 ± 0.01	0.05 ± 0.00
C22:0	0.30 ^a ± 0.00	0.43 ^b ± 0.00	0.52 ^c ± 0.00	0.43 ^d ± 0.00	0.63 ^e ± 0.00
C20:3n6	0.05 ^a ± 0.00	0.04 ^b ± 0.00	0.03 ^c ± 0.00	0.02 ^d ± 0.00	0.03 ^c ± 0.00
C22:1n9	ND	ND	0.05 ± 0.00	ND	ND
C20:4n6	0.66 ^a ± 0.00	0.37 ^b ± 0.00	0.37 ^b ± 0.00	0.18 ^c ± 0.01	0.39 ^d ± 0.00
C23:0	0.05 ± 0.01	0.04 ± 0.04	0.05 ± 0.00	0.04 ± 0.00	0.06 ± 0.00
C24:0	0.16 ^a ± 0.00	0.18 ^b ± 0.00	0.21 ^c ± 0.01	0.19 ^b ± 0.03	0.24 ^d ± 0.03
C20:5n3	0.06 ± 0.05	0.06 ± 0.05	0.18 ± 0.16	ND	0.04 ± 0.07
C24:1	0.01 ± 0.01	0.01 ± 0.01	0.03 ± 0.03	0.04 ± 0.02	0.02 ± 0.02
C22:6n3	0.31 ^a ± 0.01	0.32 ^{ab} ± 0.00	0.33 ^b ± 0.01	0.09 ^c ± 0.00	0.24 ^d ± 0.00
SFAs	42.28 ^a ± 0.05	39.23 ^b ± 0.02	29.91 ^c ± 0.03	25.57 ^d ± 0.03	22.06 ^e ± 0.02
SCFAs	0.15 ^a ± 0.00	0.17 ^b ± 0.00	0.17 ^b ± 0.01	0.15 ^a ± 0.01	0.70 ^c ± 0.32
MCFAs	14.67 ^a ± 0.04	15.21 ^b ± 0.01	16.36 ^c ± 0.02	13.98 ^d ± 0.01	3.54 ^e ± 0.01
LCFAs	27.46 ^a ± 0.01	23.86 ^b ± 0.03	13.38 ^c ± 0.02	11.44 ^d ± 0.02	17.82 ^e ± 0.02
ONSFAs	0.19 ^a ± 0.00	0.18 ^a ± 0.04	0.18 ^a ± 0.00	0.13 ^c ± 0.01	0.53 ^d ± 0.01
MUFAs	36.85 ^a ± 0.02	39.66 ^b ± 0.03	49.53 ^c ± 0.08	52.17 ^d ± 0.06	52.38 ^e ± 0.07
PUFAs	20.80 ^a ± 0.08	21.05 ^b ± 0.08	20.38 ^c ± 0.04	22.26 ^d ± 0.05	25.52 ^e ± 0.10
LA/ALA	12.06 ^a ± 0.01	7.88 ^b ± 0.02	7.99 ^c ± 0.01	10.55 ^d ± 0.01	8.86 ^e ± 0.00

^a Abbreviations are: SFAs, saturated fatty acids; SCFAs, short-chain SFAs; MCFAs, medium-chain SFAs; LCFAs, long-chain SFAs; ONSFAs, odd-chain number SFAs; MUFAs, monounsaturated fatty acids; PUFAs, polyunsaturated fatty acids; LA/ALA, linoleic acid/ α -linolenic acid. Values are means \pm standard deviation (ND, not detected); different superscript letters indicate significant differences ($P < 0.05$) within a row.

OPO-NF1–4), ranged from 16.37% to 8.21% and were significant higher than those in unsupplemented infant formulas, OPO-F2 and OPO-NF5, at 8.09% and 3.52%, respectively).

The total of lauric and myristic acids is recommended not to exceed 20% of total fat in infant formulas (Berthold et al., 2005). The results also revealed that the highest value of MCFAs in the infant formulas studied was 16.37%, so the combined concentration of lauric and myristic acids was lower than 20% of total fat, which totally meets the global standards.

With regard to LCFAs, which account for more than 60% of SFAs, the content of LCFAs in OPO-Fs (24.27–38.29%) were higher than those in OPO-NFs (11.41–27.41%) (Tables 1 and 2). Palmitic acid was the most predominant LCFA in infant formulas and human milk (above 20%; Sun et al., 2016; Zou et al., 2013). The values of palmitic acid in OPO-Fs (19.47–29.08%) were also significantly higher than those in OPO-NFs (7.65–22.13%). This reflected that with the rac-OPO supplementation the concentrations of LCFAs and palmitic acid increased.

Stearic acid (C18:0) was another predominant LCFA in infant formulas. The contents of stearic acid were also affected by different basic materials of infant formulas; compared with plant oil, milk fat contains higher concentrations of stearic acid (Orsavova, Misurcova, Ambrozova, Vicha, & Mlcek, 2015; Zou et al., 2013). The results of our study (Tables 1 and 2) also showed that infant formulas based on whole milk (OPO-F1–4, 5.94–7.85%) contained higher stearic acid levels than those infant formulas

based on skimmed milk (OPO-F5, OPO-NF1–5, 2.69–4.88%). The PCA loading plot also reflected that stearic acid was one of the variables characterising the OPO-F1–4 group (Fig. 1B).

Regarding the other LCFAs (C20:0, C22:0 and C24:0), the contents of which were <1%, these were affected by the addition of plant oil (Fig. 1A and B). The results showed that the contents of C20:0, C22:0 and C24:0 were associated with the infant formulas based on skimmed milk (Fig. 1A and B). Odd-numbered SFAs (ONSFAs; C11:0, C13:0, C15:0, C17:0 and C23:0) were also detected in infant formulas. The results showed that the levels of odd-numbered SFAs were also related to the milk fat, since infant formulas based on whole milk (OPO-F1–4) contained higher contents of ONSFAs (0.67–0.93%) than those based on skimmed milk (OPO-F5 and OPO-NF1–5; 0.13–0.53%). See Tables 1 and 2). The PCA loading plot also demonstrated that stearic acid and ONSFAs were associated with the OPO-F1–4 groups, which contained milk fat in the ingredient lists (Fig. 1B).

MUFAs were the most abundant FAs in infant formulas and human milk. The results showed that with the supplementation of rac-OPO, the concentrations of MUFAs decreased (Tables 1 and 2). The contents of MUFAs in OPO-Fs (30.02–42.31%) were significantly ($p < 0.05$) lower than those in OPO-NFs (34.49–52.37%), but similar to the levels in Chinese human milk (about 35% of total FAs; Sun et al., 2016; Zou et al., 2013).

Oleic acid was the most predominant MUFA in human milk and infant formulas. In the main, oleic acid content of OPO-Fs was lower

Table 3
TAG profiles of infant formulas in OPO-Fs.^a

TAGs	OPO-F1	OPO-F2	OPO-F3	OPO-F4	OPO-F5
MCaCa	0.25 ^a ± 0.02	0.03 ^b ± 0.02	0.07 ^c ± 0.01	0.12 ^d ± 0.03	0.42 ^e ± 0.01
MCaLa	0.22 ^a ± 0.04	0.02 ^b ± 0.01	0.07 ^c ± 0.02	0.08 ^c ± 0.02	0.26 ^d ± 0.02
LaLaLa	1.85 ^a ± 0.02	0.05 ^b ± 0.01	0.26 ^c ± 0.03	0.41 ^d ± 0.02	0.57 ^e ± 0.02
MLaLa	0.58 ^a ± 0.02	0.07 ^b ± 0.01	0.14 ^c ± 0.03	0.17 ^c ± 0.02	0.43 ^d ± 0.02
MMLa	0.54 ^a ± 0.02	0.32 ^b ± 0.02	0.17 ^c ± 0.02	0.29 ^d ± 0.03	0.22 ^e ± 0.03
LLL	7.77 ^a ± 0.02	12.10 ^b ± 0.01	10.28 ^c ± 0.03	9.17 ^d ± 0.02	7.81 ^e ± 0.02
OLL	12.34 ^a ± 0.02	8.15 ^b ± 0.03	10.66 ^c ± 0.02	11.95 ^d ± 0.04	7.23 ^e ± 0.01
PLL	5.94 ^a ± 0.03	6.17 ^b ± 0.01	3.90 ^c ± 0.02	3.37 ^d ± 0.01	6.64 ^e ± 0.02
OOL	12.26 ^a ± 0.03	5.73 ^b ± 0.01	10.44 ^c ± 0.04	11.77 ^d ± 0.07	4.12 ^e ± 0.02
OPL	8.33 ^a ± 0.04	12.60 ^b ± 0.02	8.32 ^a ± 0.03	8.66 ^c ± 0.01	8.67 ^c ± 0.01
PPL	3.03 ^a ± 0.02	5.45 ^b ± 0.03	3.55 ^c ± 0.02	4.37 ^d ± 0.04	3.55 ^c ± 0.02
OOO	14.11 ^a ± 0.01	5.26 ^b ± 0.02	15.27 ^b ± 0.01	14.59 ^c ± 0.03	30.48 ^d ± 0.01
OPO	16.15 ^a ± 0.01	20.48 ^b ± 0.01	18.69 ^c ± 0.04	17.95 ^d ± 0.01	16.89 ^e ± 0.01
PPO	11.33 ^a ± 0.01	16.92 ^b ± 0.02	12.80 ^c ± 0.08	12.70 ^c ± 0.12	10.95 ^d ± 0.03
PPP	2.30 ^a ± 0.10	3.72 ^b ± 0.01	2.84 ^c ± 0.04	2.37 ^d ± 0.06	ND
SOO	1.16 ^a ± 0.03	0.69 ^b ± 0.18	0.95 ^c ± 0.08	0.70 ^d ± 0.01	1.81 ^d ± 0.09
POS	1.87 ^a ± 0.01	2.27 ^b ± 0.02	1.62 ^c ± 0.02	1.36 ^d ± 0.02	ND

^a TAG names do not indicate positional location of fatty acids in the triacylglycerols. Abbreviations are: Ca, capric acid; La, lauric acid; M, myristic acid; P, palmitic acid; S, stearic acid; O, oleic acid; L, linoleic acid. Values are means ± standard deviation (ND, not detected); different superscript letters indicate significant differences ($P < 0.05$) within a row.

Table 4
TAG profiles of infant formulas in OPO-NFs.^a

TAGs	OPO-NF1	OPO-NF2	OPO-NF3	OPO-NF4	OPO-NF5
MCaCa	0.44 ^a ± 0.06	0.36 ^b ± 0.01	0.47 ^a ± 0.05	0.26 ^c ± 0.03	ND
MCaLa	0.25 ^a ± 0.02	0.27 ^a ± 0.03	0.27 ^a ± 0.03	0.15 ^b ± 0.02	ND
LaLaLa	1.32 ^a ± 0.01	1.11 ^b ± 0.02	ND	0.65 ^c ± 0.03	ND
MLaLa	0.47 ^a ± 0.02	0.29 ^b ± 0.03	1.31 ^c ± 0.02	0.27 ^b ± 0.02	ND
MMLa	0.26 ^a ± 0.04	0.24 ^a ± 0.02	0.46 ^b ± 0.03	0.14 ^b ± 0.01	ND
LLL	9.33 ^a ± 0.04	10.06 ^b ± 0.05	12.01 ^c ± 0.02	9.96 ^d ± 0.03	12.27 ^d ± 0.05
OLL	6.36 ^a ± 0.02	6.64 ^b ± 0.03	9.53 ^c ± 0.03	12.35 ^d ± 0.00	5.84 ^e ± 0.01
PLL	5.76 ^a ± 0.04	5.72 ^a ± 0.03	8.26 ^b ± 0.14	8.40 ^b ± 0.01	10.20 ^c ± 0.02
OOL	4.83 ^a ± 0.04	4.48 ^b ± 0.03	9.86 ^c ± 0.06	13.39 ^d ± 0.09	3.93 ^e ± 0.02
OPL	9.67 ^a ± 0.04	8.17 ^b ± 0.01	2.83 ^c ± 0.01	6.39 ^d ± 0.01	8.16 ^e ± 0.01
PPL	5.80 ^a ± 0.01	3.25 ^b ± 0.02	ND	ND	ND
OOO	19.31 ^a ± 0.02	32.43 ^b ± 0.02	50.38 ^c ± 0.04	42.61 ^d ± 0.01	51.33 ^e ± 0.18
OPO	17.66 ^a ± 0.03	12.78 ^b ± 0.00	4.66 ^c ± 0.02	5.46 ^d ± 0.01	5.15 ^e ± 0.02
PPO	16.13 ^a ± 0.01	10.07 ^b ± 0.02	ND	ND	ND
PPP	1.52 ± 0.15	ND	ND	ND	ND
SOO	0.92 ^a ± 0.01	2.60 ^b ± 0.03	ND	ND	3.14 ^c ± 0.10
POS	ND	1.58 ± 0.02	ND	ND	ND

^a TAG names do not indicate positional location of fatty acids in the triacylglycerols. Abbreviations are: Ca, capric acid; La, lauric acid; M, myristic acid; P, palmitic acid; S, stearic acid; O, oleic acid; L, linoleic acid. Values are means ± standard deviation (ND, not detected); different superscript letters indicate significant differences ($P < 0.05$) within a row.

were dispersed and positioned on the positive side of PC1. With regard to PC2, no obvious group separation was observed, except OPO-F2 and OPO-NF5 were relatively far away from the other infant formulas (Fig. 2A).

The PCA loading plot showed that PPO, OPO, PPL, PPP, POS and OPL were linked to the OPO-F1–5 and OPO-NF1–2 group (Fig. 2A). OPO-F1–5 and OPO-NF1–2 contained higher concentrations than OPO-NF3–5 of PPO, OPO, PPL, PPP, POS and OPL. In contrast, OPO-NF3–5 contained higher concentrations than OPO-F1–5 and OPO-NF1–2 of LLL, PLL and OOO. This corresponded with the results that OPO-F1–5 and OPO-NF1–2 contained higher levels of palmitic acid, while OPO-NF3–5 contained higher levels of oleic acid and linoleic acid. Most OPO contents were the highest in OPO-Fs (16.15–20.48%), except in OPO-F5, which contained higher levels of OOO (30.48%) than OPO (16.89%). OPO-NF1 and OPO-NF2 also possessed relative high levels of OPO (17.66% and 12.78%, respectively), but the content of OPO in OPO-NF3–5 ranged from 4.66% to 5.46%, far lower than in OPO-F1–5 and OPO-NF1–2 (Tables 3 and 4).

It has been reported that in human milk, the most two abundant TAGs were OPO and OPL; especially in Chinese human milk, the levels of OPL (26.83%) were higher than OPO (16.22%) (Sun et al.,

2018b). The contents of OPL in OPO-Fs ranged from 8.32% to 12.60%, and in OPO-NFs from 2.83% to 9.67%, all obviously lower than in human milk. PPO was another predominant TAG in OPO-Fs, the content of which ranged from 10.95% to 16.92% (Table 2A). It is also observed that OPO-NF1 and OPO-NF2 also contained relatively high concentrations of PPO at 16.13% and 10.07%, respectively (Table 2B). However, PPO were not detected in OPO-NF3–5 (Table 2B). PPL were also not detected in OPO-NF3–5, the contents of which in OPO-F1–5 and OPO-NF1–2 ranged from 3.03% to 5.80%. PPP were not detected in OPO-F5 and OPO-NF2–5, the contents of which in OPO-F1–4 and OPO-NF1 ranged from 1.52% to 3.32%. POS were not detected in OPO-F5, OPO-NF1,3–5, while in OPO-F1–4 and OPO-NF2 the contents of POS ranged from 1.58% to 2.27%.

For the most part, OPO and PPO contents in coconut, palm kernel, rapeseed, high oleic sunflower, sunflower, soybean and corn oil, used as supplements in the infant formulas studied, do not exceed 5% (Chai et al., 2018; Gao et al., 2017; Guan et al., 2016); however, palm and palm stearins oil possess relatively high levels of OPO and PPO, about 25% and 28%, respectively (Braisson-Danthine, 2007). Palm and palm stearins oil are usually used as raw materials to prepare OPO as human milk fat substitutes or for

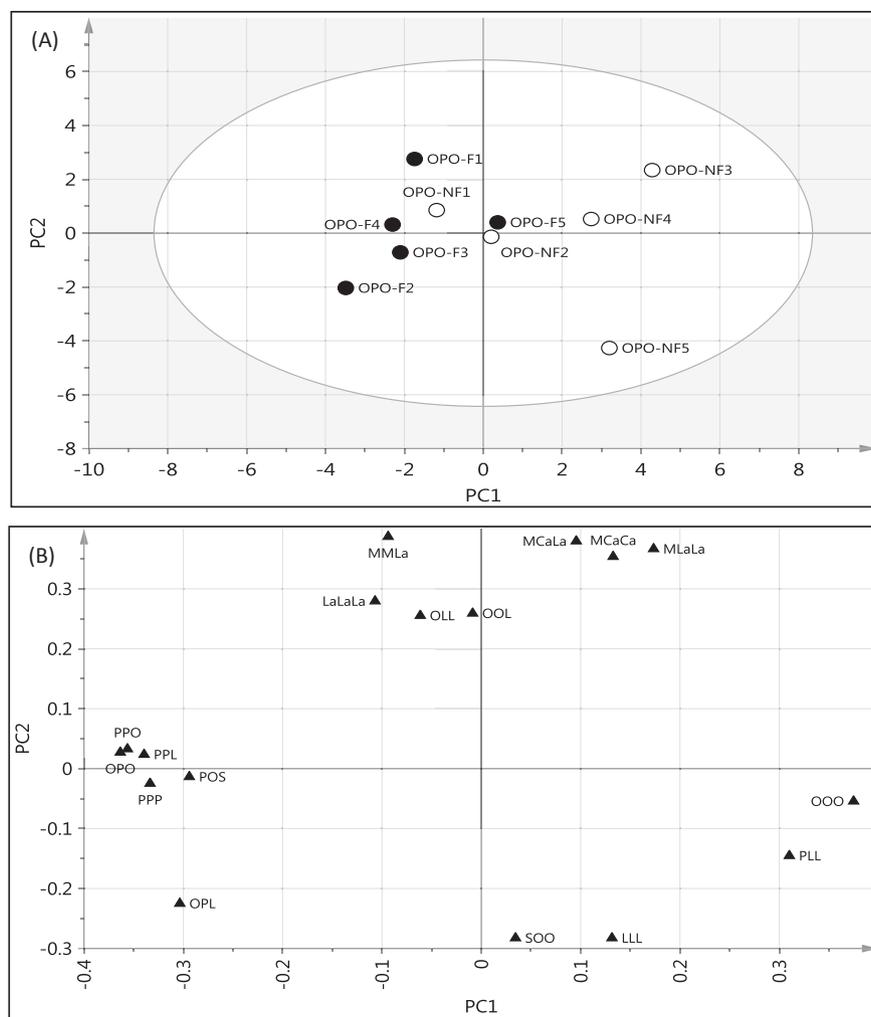


Fig. 2. PCA score scatter plot (A) and loading plot (B) of TAG profiles of OPO-Fs and OPO-NFs.

direct addition into infant formulas (Lee, Son, Akoh, Kim, & Lee, 2010; Lee, Won Oh, Kwon, & Yoon, 2015; Wei, Feng, Zhang, Cao, & Feng, 2015). The levels of OPO and PPO were mainly related to the supplementation of rac-OPO and palm or palm stearin oil. As regards OPL, this is mainly found in sunflower, corn and soybean oil, but is almost non-detectable in rapeseed oil (Gao et al., 2017; Guan et al., 2016). The relatively high levels of OPO, PPO, OPL and PPL in OPO-NF1–2 resulted from the addition of palm and palm stearin oil as shown in the ingredient lists; hence OPO-NF1–2 was close to the OPO-Fs on the PC1 vector of the PCA (Fig. 2A).

The PCA loading plot demonstrated that OOO, LLL and PLL associated with the position distribution of OPO-NF3–5 on the PC1 vector (Fig. 2A). The contents of OOO ranged from 5.26% to 30.48% in OPO-Fs, lower than in OPO-NFs (19.31–51.33%), but still higher than in human milk (approximately 2%) (Kallio et al., 2017; Sun et al., 2018b; Tu et al., 2017). OOO was the predominant TAG (above 70%) in rapeseed oil and high oleic sunflower oil, the concentrations of which were approximately 70% and 66%, respectively (Gao et al., 2017; Guan et al., 2016); in cow and goat milk the contents of OOO did not exceed 3% (Zou et al., 2013). Therefore, the high concentrations of OOO in infant formulas, especially in OPO-NFs, were related to the supplementation with rapeseed oil and high oleic sunflower oil. Table 4 shows that for the most part, the contents of LLL and PLL in OPO-NFs (7.11–12.10% and 5.76–12.10%) were also higher than in OPO-Fs (9.33–12.27% and 3.90–6.64%). It has been reported that sunflower, corn, soybean oil, which are also

commonly added into infant formulas, contain relatively high concentrations of LLL and PLL (Gao et al., 2017). In contrast, LLL and PLL can hardly be detected in rapeseed oil (Guan et al., 2016). Therefore, the levels of LLL and PLL resulted from supplementation with sunflower, corn, and soybean oil. OLL and OOL, the contents of which in rapeseed, sunflower, soybean and corn oil are all relatively high, were also main variances affecting the distribution of infant formulas in the PC2 vector (Gao et al., 2017; Guan et al., 2016). The results Tables 3 and 4 show that the content of OLL and OOL in infant formulas (5.84–12.35% and 3.93–13.39%, respectively) covered a wide range, which may relate to the different amount supplementation of plant oil in infant formulas.

The loading plot reflected that TAGs with an equivalent carbon number ≤ 40 (ECN ≤ 40), including (using the abbreviations: M, myristic acid; Ca, capric acid; La, lauric acid) MCaCa, MLaLa, LaLaLa, MLaLa, and MMLa, were linked to OPO-F1,3–5 and OPO-NF1–4, which were supplemented with palm kernel oil and coconut oil (Fig. 2B). Palm kernel oil and coconut oil contain high concentrations of LaLaLa, MLaLa, CaLaLa and MMLa (above 10%). As shown in Tables 3 and 4, the content of TAGs (ECN ≤ 40) includes MCaCa, MLaLa, LaLaLa, MLaLa, and MMLa, which contain medium-chain FAs, corresponded to the results of MCFA concentrations in infant formulas. The contents of MCaCa, MLaLa, LaLaLa, MLaLa, and MMLa in infant formulas that were supplemented with coconut oil or palm kernel oil (0.07–0.47%, 0.07–0.27%, ND–1.85%, 0.14–1.31% and 0.14–0.54%, respectively; OPO-F1,3–5 and OPO-NF1–4) were

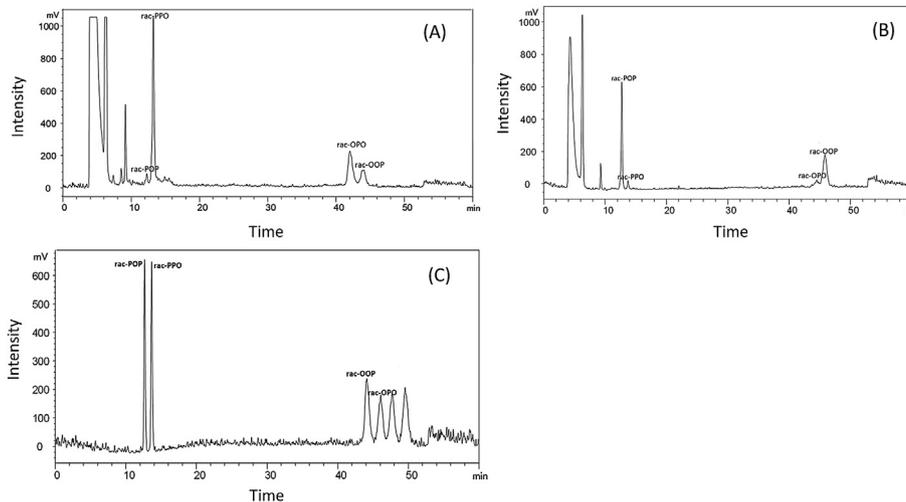


Fig. 3. Chromatograph of rac-POP/rac-PPO and rac-OPO/rac-OOP in OPO-F1(A), OPO-NF1(B) and standards samples of rac-POP/rac-PPO and rac-OPO/rac-POP (C).

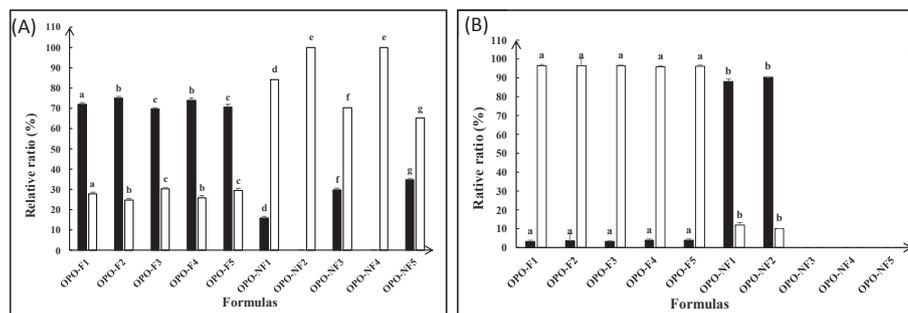


Fig. 4. The relative ratios of regioisomers of OPO (A: ■, rac-OPO; □, rac-OOP) and PPO (B: ■, rac-POP; □, rac-PPO) in OPO-Fs and OPO-NFs. Columns with different letters were significantly different at $P < 0.05$.

significantly higher than in those infant formulas (OPO-F2 and OPO-NF5) that were not supplemented. TAGs ($ECN \leq 40$) were not detected in OPO-NF5 in our study, and the contents of MCaCa, MCaLa, LaLaLa, MLaLa, and MMLa in OPO-F2 were 0.03%, 0.02%, 0.05%, 0.07% and 0.32%, respectively.

3.3. The regioisomers of rac-OPO/rac-OOP and rac-PPO/rac-POP TAGs in infant formulas

The regio-specific distribution of palmitic acid on TAGs can influence the absorption of both fat and calcium, bone health, intestinal flora and infant comfort (Miles & Calder, 2017; Petit, Sandoz, & Garcia-Rodenas, 2017; Wan et al., 2016). In human milk, more than 70% of the palmitic acid is esterified on the sn-2 position of TAGs (Zou et al., 2013). OPO and PPO were the two main TAGs that contained palmitic acid, both of which contained two regioisomers rac-OPO/rac-OOP and rac-PPO/rac-POP, respectively. rac-OPO and rac-PPO were the main regioisomers of OPO and PPO, the relative ratios of which were both above 90% (Kallio et al., 2017). In our study, the regioisomers of the relative ratios of OPO and PPO in infant formulas are presented in Fig. 4A,B; the relative ratios of rac-OPO/rac-OOP were significantly different between OPO-Fs and OPO-NFs (Fig. 3A,B). The results showed that rac-OPO was the predominant regioisomer in OPO-Fs, the relative ratios of which ranged from 69.72% to 75.11%; in OPO-NFs, rac-OOP was the predominant regioisomer of OPO. In OPO-NF1,3,5, the relative ratios of rac-OOP were 84.23%, 70.29% and 65.24%, respectively. In OPO-NF2,4, rac-OPO was not detected. The results

reflected that the relative abundance of rac-OPO in OPO-Fs was lower than that in human milk. With regard to the regioisomer PPO, rac-PPO was the predominant regioisomer of OPO-Fs, the relative ratio of which was above 95%; in OPO-NF1–2, rac-POP was the predominant regioisomer, relative ratios of which were 88.18% and 90.34%, respectively. Although high levels of OPO and PPO may be observed in OPO-NFs, the regioisomers were significantly different from those in OPO-Fs and human milk, which reflected that in plant oil palmitic acid were mainly esterified at the sn-1/3 position, not the sn-2 position. Therefore, significant effort is still needed for infant formulas to mimic human milk.

4. Conclusions

Different fat ingredients in infant formulas resulted in significant differences of FAs and TAGs composition. The addition of rac-OPO (OPO-F5), palm and palm stearins oil (OPO-NF1–2) in infant formulas improved the levels of SFAs (37.77–47.88%), mainly palmitic acid (19.47–29.08%), and TAGs included PPO (10.07–16.92%), OPO (12.78–20.48%), PPL (3.03–5.80%), PPP (ND–3.72%), POS (ND–2.27%) and OPL (8.17–12.60). However, although similar levels of palmitic acid and PPO and OPO were seen in OPO-Fs and OPO-NFs, the regioisomers of OPO and PPO were significantly different. The predominant regioisomers of OPO and PPO in OPO-Fs were rac-OPO (approximately 70%) and rac-PPO (above 95%), while in OPO-NFs were rac-OOP (65.24–100%) and rac-POP (about 90%). The supplementation of plant oil, mainly rapeseed and high oleic sunflower oil, in infant formulas strongly enhanced the contents of

oleic acid and OOO, which were observed in OPO-NFs, especially OPO-NF3–5 (48.79–51.62% and 42.61–51.33%, respectively). The supplementation of milk fat in infant formulas (OPO–F1–4) resulted in high concentrations of SCFAs (1.07–1.46%), stearic acid (5.94–7.85%), ONSFAs (0.67–0.93%), myristoleic (0.21–0.35%) and palmitoleic acid (0.39–0.59%). Coconut and palm kernel oil enhanced the levels of MCFAs (16.37–8.21%) and TAGs, including MCaCa (0.07–0.47%), MCaLa (0.07–0.27%), LaLaLa (ND–1.85%), MLaLa (0.14–1.31%) and MMLa (0.14–0.54%) (in OPO–F1,3–5 and OPO–NF1–4).

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