Data Article

Quantitative determination of conjugated linoleic acid and polyunsaturated fatty acids in milk with C17:0 as internal marker – Evaluation of different methylation procedures

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ARTICLE INFO

ABSTRACT

Fatty acids are commonly analysed by gas chromatography as their corresponding fatty acid (FA) methyl esters (FAME). For quantitative determination of individual FA an internal standard like C17:0 is necessary. Conjugated FA and polyunsaturated fatty acid (PUFA) represents a challenge in the methylation steps, as they are sensitive to pH changes and oxidation. The present study was carried out to determine the efficiency of different methylation procedures on quantitative determination of conjugated linoleic acid (CLA), PUFA and response of internal standard. The highest response of internal standard was observed for boron trifluoride (BF_3)/ methanol and methanolic HCl followed by $NaOCH_3$, while cis-9, trans-11 CLA, total CLA and PUFA was higher with methanolic HCl followed by $NaOCH_3$ compared with the BF_3 method. These data can be useful for quantitating of milk FA.

Specifications Table

Subject area	*Analytical chemistry, food chemistry*
More specific subject area	*Milk fatty acid methylation and analysis*

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Type of data	*Tables*
How data was acquired	*Gas chromatograph (Hewlett-Packard 6890 series, Agilent Technologies, Palo Alto, CA, USA) equipped with an automatic column injector (Hewlet Packard 7673), a capillary column of 30 m × 0.32 mm i.d., 0.25 µm thickness (Omegawax 320; Supelco, Sigma- Aldrich), and a flame ionization detector.*
	The initial temperature was set at 60 °C, and then the temperature was raised to 210 °C at the rate of 2 °C/min.
	Fatty acids were identified by comparison of retention times with external standards (GLC-68C, Nu- Prep-Check, Elysian, MN, USA).
Data format	*Raw data collection and analysis.*
Experimental factors	*Evaluation of different methylation procedures for quantitative analyses of CLA, PUFA and C17:0 as internal standard including: alkaline catalysts, acidic catalysts and combination of alkaline and acidic catalysts.*
Experimental features	*Obtained data were analyzed in a completely randomized design*
Data source location	*Aarhus university, AU Foulum, DK-8830 Tjele, Denmark*
Data accessibility	*Data are presented in this article*

Value of the data

- Despite all various methods employed for milk FA analyses, there are still conflicting opinions about the best method for overcoming all the difficulties posed by the analysis of complex mixtures including CLA isomers and PUFA.
- For quantitative analysis of FA, addition of internal standard is necessary. Furthermore, when an internal standard is used, the method has the capability to determine both total FA distribution and the amount of individual FA in a given sample simultaneously.
- Due to the heterogeneity of milk fatty acid, it is necessary to study the methylation procedure in order to obtain accurate quantitative and qualitative results.

1. Data

The internal standard response was checked to verify the effect of different methylation procedures on methylation of internal standard. Table 1 shows area under the chromatogram peak of C17:0 analyzed following the different methylation methods. The area under the chromatogram peaks was 2706 and 1834 units for the C17:0 methylated with BF_3/methanol and methanolic HCl followed by $NaOCH_3$ procedures, respectively. However, response of internal standard for the other methods was near to zero. In the present study, methanolic HCl followed by $NaOCH_3$ and BF_3/methanol methods catalyzed methylation of C17:0; therefore, analysis of milk samples with these two methods was included in the paper. Table 2 shows milk FA amount and composition following the two methylation procedures. The amount of total FA for BF_3/methanol method was 95% of the amount detected with the methanolic HCl followed by $NaOCH_3$ method. Cis-9, trans-11 CLA was 29% higher with methanolic HCl followed by $NaOCH_3$ than the BF_3/methanol method. In addition, with methanolic HCl followed by $NaOCH_3$, amount of trans-10, cis-12 CLA was 23% higher than with the BF_3/methanol method.