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Fatty Acid Prediction in Bovine Milk by Attenuated Total Reflection Infrared Spectroscopy after Solvent-Free Lipid Separation

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Citation: Akhgar, C.K.; Nürnberger, V.; Nadvornik, M.; Velik, M.; Schwaighofer, A.; Rosenberg, E.; Lendl, B. Fatty Acid Prediction in Bovine Milk by Attenuated Total Reflection Infrared Spectroscopy after Solvent-Free Lipid Separation. *Foods* **2021**, *10*, 1054. https://doi.org/10.3390/foods10051054

Academic Editors: Ben Aernouts, Clement Grelet and Ines Adriaens

Received: 30 March 2021
Accepted: 10 May 2021
Published: 11 May 2021

Abstract: In the present study, a novel approach for mid-infrared (IR)-based prediction of bovine milk fatty acid composition is introduced. A rapid, solvent-free, two-step centrifugation method was applied in order to obtain representative milk fat fractions. IR spectra of pure milk lipids were recorded with attenuated total reflection Fourier-transform infrared (ATR-FT-IR) spectroscopy. Comparison to the IR transmission spectra of whole milk revealed a higher amount of significant spectral information for fatty acid analysis. Partial least squares (PLS) regression models were calculated to relate the IR spectra to gas chromatography/mass spectrometry (GC/MS) reference values, providing particularly good predictions for fatty acid sum parameters as well as for the following individual fatty acids: C10:0 (R^2_P = 0.99), C12:0 (R^2_P = 0.97), C14:0 (R^2_P = 0.88), C16:0 (R^2_P = 0.81), C18:0 (R^2_P = 0.93), and C18:1cis (R^2_P = 0.95). The IR wavenumber ranges for the individual regression models were optimized and validated by calculation of the PLS selectivity ratio. Based on a set of 45 milk samples, the obtained PLS figures of merit are significantly better than those reported in literature using whole milk transmission spectra and larger datasets. In this context, direct IR measurement of the milk fat fraction inherently eliminates covariation structures between fatty acids and total fat content, which poses a common problem in IR-based milk fat profiling. The combination of solvent-free lipid separation and ATR-FT-IR spectroscopy represents a novel approach for fast fatty acid prediction, with the potential for high-throughput application in routine lab operation.

Keywords: mid-infrared spectroscopy; attenuated total reflection; bovine milk; fatty acids; partial least squares

1. Introduction

Milk is among the fastest growing agricultural commodities, with a worldwide production volume of more than 8.5×10^6 tons per annum, and an expected yearly growth rate of 1.6% until 2029 [1]. Bovine milk accounts for approximately 81% of total milk production, and is considered to be one of the most nutritionally complete foods, with a typical gross composition of 3.9% fat, 3.3% protein, and 4.6% lactose [2]. Milk fat predominantly consists of triglycerides, containing more than 400 different fatty acids,