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NEAR INFRARED SPECTROSCOPY FOR THE QUALITY ASSESSMENT OF DAIRY PRODUCTS

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1. INTRODUCTION

The dairy industry has experienced significant technological advancements and growth in recent decades, driven by increasing consumer demand for safe, nutritious, and high-quality products (Barkema et al., 2015; Di Rosa et al., 2017). Food quality is defined by traceable origin, chemical composition, physical characteristics, sensory evaluation, and safety measures regarding microbiological and toxicological properties, all of which are influenced by processing and storage (Hew et al., 2024; Ray, 2023). Ensuring quality has led to the development of efficient analytical methods to support fair competition and protect consumers.

Global milk production is projected to reach 981 million metric tons by 2028, growing at 1.7% annually, with consumption rising especially in low-income, densely populated regions where milk serves as a primary protein source (Bista et al., 2021; Sager et al., 2018). Challenges such as perishability, transportation, and inadequate refrigeration have prompted processing methods like evaporation and drying to produce milk powders (Wang et al., 2021; Kapaj & Deci, 2017; Zouari et al., 2019). While liquid milk has a

creamy texture and short shelf life suitable for immediate consumption and beverages, powdered milk offers extended shelf life and versatility in industrial applications, including ice cream, yogurt, chocolate, baked goods, and sauces (Zouari et al., 2020; Pugliese et al., 2017; Tirgarian et al., 2023; Augustin et al., 2003).

Milk powder quality depends on chemical, physical, and functional properties, including protein behavior under varying pH and temperature, amino acid composition, insolubility index, titratable acidity, and fat content (Schuck, 2011; Sutariya et al., 2017). Nutritional factors like amino acids are critical for infant formulas, while fat content affects shelf life and functionality (Sharma et al., 2012; Hoppe et al., 2008).

Milk fat, containing over 400 fatty acids, including CLA and omega-3 PUFAs, is crucial for nutritional, physical, and sensory attributes (Kholif & Olafadehan, 2022; Kokić et al., 2024; Tóth et al., 2019). These fatty acids support cardiovascular health, reduce inflammation, and enhance immune function (Shahidi & Ambigaipalan, 2018; Gebreyowhans et al., 2019). Milk fat composition is influenced by breed, season, lactation stage, and diet, which

can be optimized through feeding strategies like supplementation with oils, oilseeds, or marine lipids, and adjusting feed-to-concentrate ratios (Magan et al., 2021; Lerch et al., 2015; Bodkowski et al., 2024).

Fermented products such as yogurt and cheese are influenced by raw milk composition, fermentation conditions, and starter cultures, with quality and shelf life highly sensitive to these parameters (Rațu et al., 2023; Alvarez-Hess et al., 2024). Authenticating the origin of raw and fermented products is particularly critical for high-value certified items such as organic, Protected Designation of Origin (PDO), Protected Geographical Indication (PGI), and Traditional Specialty Guaranteed (TSG) dairy products (Chaudhary et al., 2022).

Dairy research integrates chemistry, physics, microbiology, and enzymology to improve milk quality, livestock nutrition, disease control, and functional product formulation (Priyashantha & Vidanarachchi, 2024; Moatsou, 2024). Milk is a complex biological system, and inappropriate treatments can destabilize it, causing defects (Nasralla et al., 2022). Analytical techniques, including chromatography and molecular methods, ensure authenticity but are often time-

consuming and require skilled operators (Coppa et al., 2015; Haider et al., 2024).

Near-Infrared Spectroscopy (NIRS) is a versatile, non-destructive technique that measures molecular vibrations of biological samples including milk and dairy products (Yang et al., 2020). Available in benchtop, portable, and handheld formats, NIRS is applied for adulteration detection, authentication, and compositional analysis, including water addition, non-dairy fat substitution, and origin verification (Yakubu et al., 2022; Hebling e Tavares et al., 2022; de la Roza-Delgado et al., 2017). Despite extensive research on raw milk, gaps remain in applying NIRS to fermented products, reconstituted milk, and non-traditional milk sources like camel and mare milk, particularly in assessing dietary effects on chemical and sensory properties. Addressing these gaps could expand NIRS's role in improving dairy quality, authenticity, and safety.

2. OBJECTIVES

The main objective of this research was to explore the potential of NIRS in identifying and addressing quality deviations/differences across selected dairy food matrices. To

achieve this goal, we have established specific research aims designed to systematically investigate and demonstrate the capabilities of NIRS:

1. **Evaluation of the quality of reconstituted cow, camel and mare milk samples using NIRS and chemometric techniques:**

The aim was to thoroughly characterize reconstituted milk samples derived from different animal sources, such as cows, mares, and camels. This involved developing robust prediction models to accurately assess critical quality parameters such as composition and functional attributes. Additionally, the aim was to create classification models to differentiate between the reconstituted milk based on their spectral profiles. This included distinguishing among the milk samples originating from different species as well as identifying variations arising from diverse reconstruction conditions. By integrating these models, we sought to ensure accurate identification and quality assessment of reconstituted milk, thereby enhancing product standardization and authenticity verification. This focused approach aimed to demonstrate the versatility and efficacy of NIRS in addressing challenges related to dairy product

quality while expanding its application to lesser-studied matrices such as mare and camel milk.

2. **Identifying key factors that distinguish fermented milk based on feeding type and probiotic potential with e-nose and NIRS techniques:**

The aim was to create robust models for fermented milk samples, classified by feeding type and probiotic potential, using data from two distinct techniques: NIRS and e-nose. Additionally, the aim was to identify the key sensors and specific wavelengths that contributed the most to the performance of the classification models. By identifying these factors, we aimed to achieve a better understanding of two key aspects: (1) the difference in the volatile profile and chemical composition between control and experimental fermented milk samples, regardless of the fermentation strain. This enabled a better understanding of how fermentation impacts milk composition independent of the probiotic strain. (2) The strain-specific variations in the chemical and volatile profile between control and experimental samples. This allowed to explore how each probiotic strain uniquely affects the milk's molecular changes and volatile compounds.

3. Evaluation of the impact of cattle feed on cheese ripening process by NIRS

Our objective was to evaluate how cow diets affect cheese ripening using NIRS to track chemical changes over 12 weeks. We developed classification models to account for feeding type and ripening duration, while identifying key wavelengths influencing model performance. This analysis aimed to (1) understand how dietary changes shape cheese characteristics and (2) reveal feed-specific effects on molecular changes in fresh cheese.

3. MATERIALS AND METHODS

3.1. Evaluation of the quality of reconstituted cow, camel and mare milk samples using NIRS and chemometric techniques

Three commercially available milk powders were used: skimmed cow milk powder (Tutti, Hungary), whole camel milk powder (Saumal, Kazakhstan), and mare milk powder (Sydyk, Kazakhstan). Powders were reconstituted with Milli-Q water at three concentrations (5%, 10%, 12.5%) and three temperatures (25 °C, 40 °C, 65 °C), with three replicates per combination, yielding 81 samples. The concentration and temperature levels were selected based on manufacturer guidelines and their suitability for accurate NIRS analysis. Samples were mixed for six minutes and stored at 4 °C until analysis (Figure 1).

Milk powders were characterized for water activity, loose bulk density, insolubility index, and amino acid profile. Water activity was measured at 25 °C (Novasina LabMaster-aw neo), loose bulk density by powder weight per volume, and insolubility index following Pugliese et al. (2017). Amino acids were quantified after hydrolysis with 6 M HCl at 110 °C for 24 h using an Automatic Amino Acid Analyzer AAA400 with post-column ninhydrin derivatization.

Reconstituted milk samples were analyzed using NIRS (400–2500 nm, XDS Rapid Content Analyzer, Metrohm, Denmark) in transflectance mode. Additional quality parameters included dry matter (oven-dried at 105 °C), pH and conductivity (Mettler Toledo SevenMulti), titratable acidity (Soxhlet–Henkel method), viscosity (MCR302 rheometer), fat content (Gerber method, ISO 2446/IDF 105), and color (ColorLite sph 850, CIE L*, a*, b*).

Statistical analysis was performed with SPSS 27 using descriptive statistics and two-way ANOVA (factors: milk type, concentration, temperature), with post hoc Tukey or Games–Howell tests. NIRS data were processed in R (v4.3.1) using aquap2, applying PCA, PCA-LDA, PLSR, and SVR on the 1100–1850 nm range. PCA-LDA classified milk type, concentration, and temperature, while PLSR predicted quality parameters. Leave-one-repeat-out cross-validation was used for model validation, with two-thirds of data for training and one-third for testing. Spectral pretreatments, including MSC, SNV, Savitzky–Golay second derivative, and de-trending, were applied to reduce noise, with the optimal method selected for final models.

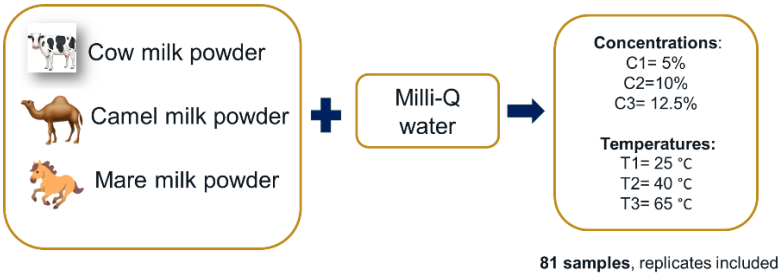

Figure 1. liquid milk samples prepared from cow, camel and mare powders

3.2 Identifying key factors that distinguish fermented milk based on feeding type and probiotic potential with e-nose and NIRS techniques

Three six-week feeding trials were conducted to evaluate the effects of Total Mixed Ration (TMR) diets supplemented with polyunsaturated fatty acids (PUFAs) compared to control diets rich in saturated fatty acids (SFAs). Each trial included 70 Holstein cows, paired by lactation number, days in milk, prior milk yield, composition, and somatic cell count, and randomly assigned to experimental or control groups. Bulk milk samples were collected weekly, with the final two weeks used for fermentation studies, yielding twelve raw milk samples, stored at 4 °C until analysis.

Fermentation used three Lactobacillus bulgaricus strains (S06, S09, S04) classified as probiotic, moderate, or non-

probiotic based on growth, bile salt tolerance, and acid resistance. Strains were activated in reconstituted skim milk at 37 °C for 24 h. Milk samples were pasteurized at 63 °C for 30 min, inoculated with 0.2 mL bacterial suspension per 200 mL, and incubated at 37 °C for 13 h. Triplicate preparations yielded 144 samples, including 108 fermented and 36 fresh milk samples (Figure 2).

Raw milk fatty acid profiles were analyzed via lipid extraction (Folch et al., 1957), formation of fatty acid methyl esters, and gas chromatography (Shimadzu Nexis 2030, FID) with a Zebron ZB-WaxPlus column, expressed as % total FAMEs. Fermented samples were analyzed using NIRS (400–2500 nm, XDS Rapid Content Analyzer, Metrohm) and e-nose (Heracles Neo 300, Alpha MOS) for chemical composition and volatile compounds. NIRS used 1.5 mL samples in 0.5 mm path vessels, three scans at 0.5 nm resolution. E-nose analyses involved headspace generation at 50 °C, dual-column GC-FID detection, and odor fingerprinting.

Data analysis included one-way ANOVA for fatty acid content (IBM SPSS 27), with normality confirmed via Anderson-Darling and Shapiro-Wilk tests. Chemometric

analyses of NIRS and E-nose data were performed in R (v4.3.1, aquap2), using PCA for outlier detection and dimensionality reduction, followed by PCA-LDA for classification by feeding type and bacterial strain. Key wavelengths and influential sensors were identified through weighted PCA-LDA loadings, with corresponding volatile compounds determined using AroChemBase v8, providing insight into chemical and sensory differences between groups.

Figure 2. Preparation of the fermented milk samples from the feeding trials

3.3. Evaluation of the impact of cattle feed on cheese ripening process by NIRS

Control and experimental Trappista cheese samples were sourced from ADEXGO Kft., produced using milk from control and experimental feeding trials (Trials 1–3). A total

of 205 fresh cheese samples were vacuum-sealed and stored at 4 °C, with 108 additional samples monitored over 0, 4, 8, and 12 weeks at 4–10 °C to assess storage effects. All experiments were performed twice to ensure reproducibility. Fresh cheese samples were analyzed for dry matter, crude fat, crude protein, and ash using standard AOAC methods. Crude fat was determined via Soxhlet extraction, crude protein via Kjeldahl digestion with ammonia titration (conversion factor 6.38), ash by muffle furnace incineration at 550 °C, and dry matter by oven drying at 105 °C until constant weight (Figure 3).

For NIRS analysis, cheese was cut into 1 cm-thick circular slices using a 3D-printed guide for uniformity. Fresh samples were scanned using a MicroNIR 1700 EC spectrometer (908–1676 nm, diffuse reflectance), while aged samples were analyzed using an XDS Rapid Content Analyzer (400–2500 nm, transflectance). All samples were scanned in random order with 3–6 replicates per sample, maintaining 20–24 °C to prevent spectral distortion due to moisture variations.

Data analysis included one-way ANOVA (IBM SPSS 27) to evaluate differences in dry matter, crude fat, protein, and ash

among feeding groups, with normality verified by the Kolmogorov-Smirnov test and significance at $p < 0.05$. Chemometric analysis of NIRS spectra was performed in R (v4.3.1, aquap2) using PCA and PCA-LDA. Spectral pretreatments included MSC, Savitzky-Golay second derivative, and de-trending. PCA-LDA models classified fresh cheese by feeding type and aged cheese by feeding type and ripening period (4, 8, 12 weeks), with models validated via threefold cross-validation. Key wavelengths contributing to classification were identified to provide insight into the chemical basis of sample differentiation.

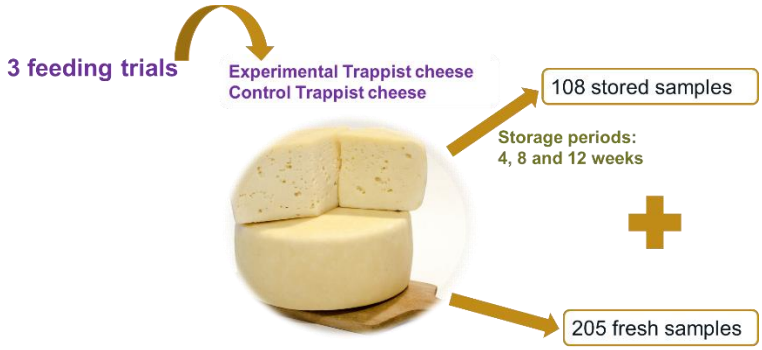

Figure 3. Preparation of the stored Trappist cheese samples

4. RESULTS

4.1. Evaluation of the quality of reconstituted cow, camel and mare milk samples using NIRS and chemometric techniques

Water activity, insolubility index, and bulk density were key indicators of milk powder quality. Cow, camel, and mare milk powders exhibited low water activity (0.22–0.28), ensuring microbial stability and long shelf life. Insolubility indices ranged from 0.1 mL (skimmed cow milk) to 1.37 mL (mare milk), reflecting protein aggregation and Maillard reaction effects during storage. Bulk density varied from 393.65 to 678.9 kg/m³, affecting packaging, handling, and flowability. These findings align with prior studies (Pugliese et al., 2017; Wang et al., 2021), confirming that milk type is a primary determinant of powder quality, influenced by processing, breed, and animal physiology.

In reconstituted milk, physicochemical properties were shaped by milk type, concentration, and temperature. Milk type most strongly affected pH, titratable acidity, and color, while concentration mainly influenced viscosity and dry matter. Camel milk had the lowest pH and highest titratable acidity, whereas viscosity increased with concentration across all types, with cow and camel milk showing the

highest values. These trends are consistent with previous reports (Swelum et al., 2021), emphasizing that milk powder source is critical in achieving consistent product characteristics.

Near-infrared spectroscopy revealed distinct spectral patterns for each milk type, with key water, fat, lactose, amino, and aromatic absorption bands enabling precise discrimination. PCA-LDA models successfully classified samples by type and concentration (Figure 4), with temperature discrimination most effective for camel milk. PLSR and SVR models accurately predicted physicochemical properties and amino acid content, with SVR generally outperforming PLSR, particularly for essential amino acids like lysine, leucine, and phenylalanine. These results demonstrate the robustness of NIRS combined with chemometric models for rapid, non-destructive quality assessment.

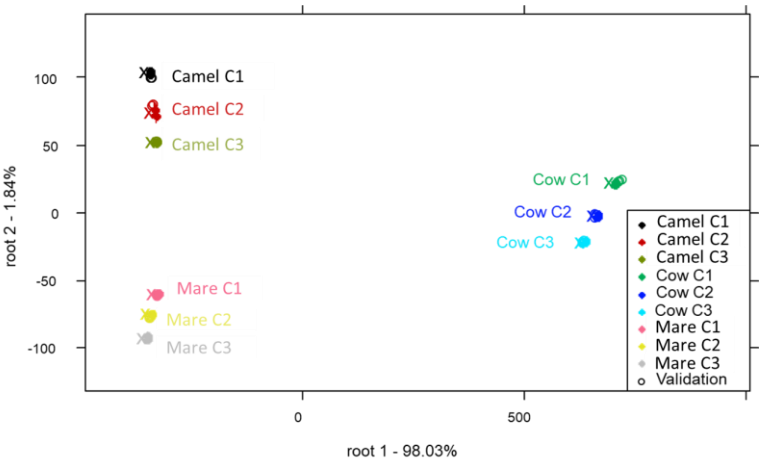

Figure 4. PCA-LDA of reconstituted milk samples at 65°C (T3) according to the concentration level on an MSC-treated spectra; C1(5%), C2(10%), C3(12.5%)

The significance of these findings lies in their practical and nutritional implications. Accurate classification and prediction of milk powder quality and composition can inform industrial quality control, optimize reconstitution procedures, and ensure nutritional adequacy in high-value products such as infant formulas. Economically, powders with controlled bulk density and solubility reduce storage and transport costs, while health-wise, precise amino acid prediction supports formulation for vulnerable populations. Compared to prior studies, this work confirms and extends the utility of NIRS and chemometric approaches for multi-

species milk analysis, offering a reliable method for industry adoption and enhancing consumer safety and product consistency.

4.2. Identifying key factors that distinguish fermented milk based on feeding type and probiotic potential with e-nose and NIRS techniques

Dietary supplementation clearly influenced the fatty acid composition of milk. In trials 1 and 2, experimental milk showed significant increases in polyunsaturated fatty acids (PUFAs) compared to controls, while saturated (SFA) and monounsaturated fatty acids (MUFA) remained largely unchanged. This reflects the effective transfer of linseed- and algae-derived PUFAs into milk fat, bypassing ruminal biohydrogenation through natural protective barriers. In trial 3, a diet enriched with linseed, linseed oil, algae extract, and fish oil led to decreased SFA and increased MUFA and PUFA levels, demonstrating that tailored feed strategies can substantially improve milk nutritional quality. These findings align with prior studies showing that dietary unsaturated fats are selectively incorporated into milk, whereas SFA levels are more resilient due to mammary de novo synthesis and rumen metabolism.

Fermented milk analysis using NIRS and e-nose further distinguished control and experimental samples. NIR spectra identified absorption bands associated with water, proteins, and fats, with key wavelengths (1164–1210 nm, 1300–1600 nm, and 1600–1800 nm) serving as markers for unsaturated fatty acids and strain-specific chemical changes. PCA-LDA models classified samples by feeding type and probiotic strain with 97–99% accuracy (Figure 5). The e-nose detected strain-specific volatile compounds, esters, diketones, aldehydes, ketones, and alcohols, which were more abundant in experimental milk enriched with unsaturated fatty acids. These compounds, together with the spectral markers, not only enabled differentiation between milk types but also enhanced sensory qualities such as fruity, buttery, and fresh aromas.

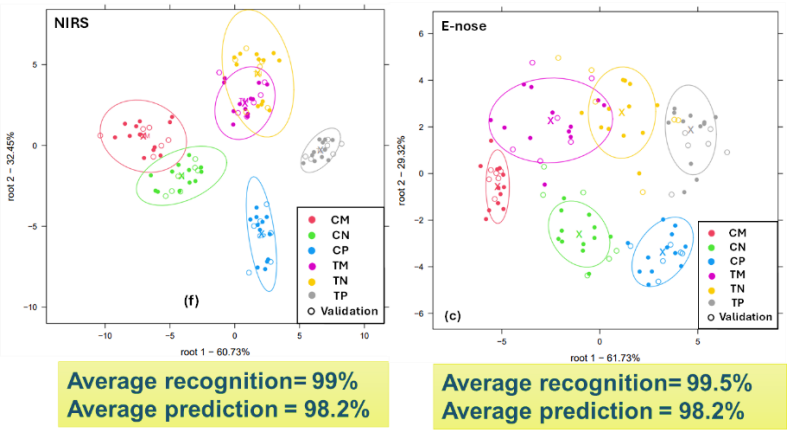

Figure 5. PCA-LDA models for experimental and control fermented milk samples from the third feeding, in the case of data points derived from the NIRS (f) and e-nose (c)

These findings demonstrate that targeted dietary interventions can effectively enhance the nutritional and sensory quality of milk, with clear benefits for human health, including improved intake of beneficial unsaturated fatty acids. The use of NIRS and e-nose technologies provides rapid, non-destructive tools to monitor milk composition and fermentation, supporting precision feeding and probiotic strategies. Specific wavelengths and virtual sensors, such as 1164–1210 nm for unsaturated fatty acids and sensors detecting key volatiles like 1-hexen-3-one, 1-hexen-3-ol, and (Z)-4-heptenal, were critical in distinguishing experimental from control samples. These markers highlight the direct

impact of dietary supplementation and microbial activity on milk's chemical and sensory profiles. For the dairy industry, this enables production of functional and differentiated products with higher market value, while also informing economic decisions on feed formulation. Compared to existing literature, these results underscore the potential of integrating advanced analytical techniques with nutritional strategies to optimize both the health profile and sensory properties of dairy products.

4.3. Evaluation of the impact of cattle feed on cheese ripening process by NIRS

Compositional analysis showed that feed supplementation with PUFA-rich sources influenced fresh cheese properties. Across three trials, crude fat consistently increased in experimental cheeses, while dry matter, protein, and ash varied depending on trial conditions, reflecting changes in moisture, protein structure, and mineral content. NIRS spectra highlighted key absorption bands for lipids (1160–1220 nm), proteins (1480–1500 nm), and water (1380–1450 nm). PCA-LDA classification models effectively distinguished control and experimental cheeses with 92–99% accuracy. Contributing wavelengths (Figure 6) varied by trial: water absorption dominated in Trial 1 (1450 nm), while

fat and fatty acids were the primary markers in Trials 2–3 (1160–1220 nm), with proteins playing a secondary role (1480–1500 nm).

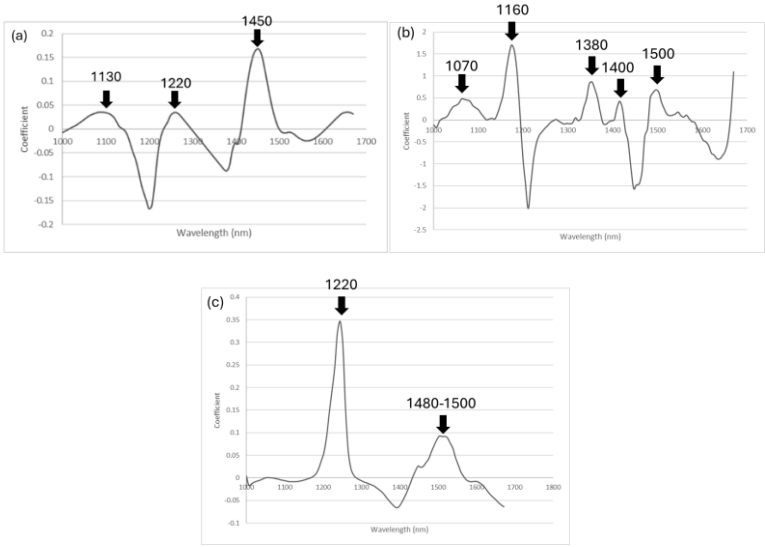

Figure 6. Contributing wavelengths to the discrimination of fresh cheese samples from trial 1 (a), trial 2 (b) and trial 3 (c), based on the type of feeding

Ripened cheeses were classified across 4, 8, and 12 weeks of storage using NIRS and LDA models, achieving up to 100% recognition and prediction accuracy. Contributing wavelengths reflected dynamic changes in water, protein, and fatty acids during ripening. Early ripening (4 weeks) was

driven by unsaturated fatty acids (1712–1726 nm), water (1380–1450 nm), and proteins, whereas by 12 weeks, saturated fatty acids (1770 nm) dominated due to oxidation, and unsaturated fatty acid contributions decreased. Water- and protein-related bands (1380–1550 nm) were consistently important across ripening, reflecting matrix and hydration changes.

These findings confirm that PUFA supplementation induces measurable molecular changes in cheese, detectable via NIRS. Compared to literature, the observed increases in unsaturated fatty acids and corresponding spectral signatures align with prior studies on feed influence on milk fat composition. The implications are broad: nutritionally, cheeses with higher PUFA content may support cardiovascular health; economically and industrially, rapid NIRS-based classification allows quality control and differentiation of functional dairy products, facilitating market adoption and premium product labelling.

5. CONCLUSIONS AND SUGGESTIONS

This research demonstrates the robust potential of near-infrared spectroscopy (NIRS) as a versatile analytical tool for characterizing dairy products, spanning reconstituted milk

powders, fermented milk, and cheese. Collectively, the three studies highlight NIRS's ability to detect compositional and biochemical variations, classify products, and provide insights relevant for both research and industry applications.

In the first study, NIRS combined with chemometric modelling effectively distinguished cow, camel, and mare milk powders, accounting for variations in concentration and reconstruction temperature. PCA-LDA models achieved 100% classification accuracy, while SVR models accurately predicted key parameters including pH, viscosity, dry matter, fat content, conductivity, and amino acids, outperforming PLSR models. These findings underscore NIRS's rapidity, minimal sample preparation, and high precision, offering valuable applications in quality control, formulation optimization, and monitoring processing conditions.

The second study explored fermented milk, integrating NIRS and electronic nose (e-nose) analyses to assess the influence of cow feeding and probiotic activity. NIRS effectively captured broad chemical attributes, while the E-nose provided sensitive detection of volatile flavor compounds. Together, these tools identified critical markers such as hexanal and 1-hexen-3-one, and NIRS wavelengths (1600–

1800 nm) revealed fatty acid profiles that differentiated milk by feeding type. This study demonstrates how combining spectral and volatile analyses can guide the development of dairy products tailored for nutritional, flavor, and probiotic properties.

The third study evaluated the effect of PUFA-rich feed on cheese composition and ripening dynamics. Crude fat content consistently increased in supplemented cheeses, while protein, dry matter, and ash showed trial-specific variations. Spectral analysis revealed key wavelengths reflecting water, protein, and fatty acid transformations during ripening. Unsaturated fatty acids dominated early stages but declined by 12 weeks due to oxidation, whereas saturated fatty acids increased. PUFA supplementation produced distinct molecular signatures, enhancing both nutritional quality and classification potential.

Together, these studies demonstrate NIRS as a rapid, non-destructive, and reliable tool for monitoring compositional changes, differentiating products, and tracking biochemical transformations across dairy matrices. The research advances dairy science by establishing a framework for spectral

fingerprinting and functional characterization of milk and cheese, supporting nutritional, health, and quality objectives.

The findings have broad relevance for nutrition, health, and industry adoption. PUFA-enriched dairy products may improve cardiovascular and metabolic health, while NIRS-based monitoring enables efficient quality control and product standardization. Economically, the rapid classification and predictive capabilities can optimize production and reduce losses. Future research should expand calibration datasets, integrate advanced chemometric approaches, and combine NIRS with complementary techniques like e-nose or mass spectrometry, further enhancing predictive accuracy, model robustness, and the sustainable production of high-quality dairy products.

6. NEW SCIENTIFIC RESULTS

The scientific findings presented here are grounded in clearly defined dairy product origins and types, as well as carefully controlled instrumental setups. For the benchtop near infrared spectroscopy (NIRS) analysis the XDS Rapid Content Analyzer (XDS RCA) (Metrohm, Herisau, Switzerland) was utilized using a circular cuvette with 0.5 mm layer thickness for reconstituted and fermented milk samples and 1 cm for stored cheese samples, respectively. The handheld device used was the MicroNIR 1700 EC spectrometer (Viavi Solutions Inc., Chandler, AR, USA), which operates in diffuse reflectance mode with a circular glass cuvette optimized for NIRS, employing a 1 cm sample thickness for fresh cheese samples. The instrumental odour analysis of the fermented milk samples was performed with the Heracles 300 ultra-fast GC analyser (Alpha MOS, Toulouse, France).

1. Combined statistical and chemometric analyses were used to characterize and predict the quality of reconstituted milk from different species. analysis of variance (ANOVA) and principal component analysis based linear discriminant analysis (PCA-LDA) models effectively distinguished cow, camel, and mare milk samples reconstituted from powders at

specific concentrations (C1 = 5%, C2 = 10%, C3 = 12.5%) and temperatures (T1 = 25 °C, T2 = 40 °C, T3 = 65 °C) with significant differences in case of main quality parameters such as the viscosity, dry matter content, titratable acidity, conductivity, pH and the colour components L*, a*, b* ($p \leq 0.05$) and 100% classification accuracy in case of NIRS, respectively. Support vector regression (SVR) models demonstrated superior predictive performance ($R^2pr = 0.80–0.99$) compared to partial least squares regression (PLSR) for the main quality parameters and amino acid profile of milk.

2. NIRS and e-nose based principal component analysis–linear discriminant analysis (PCA-LDA) models were developed to distinguish fermented milk obtained from cows fed either a Total Mixed Ration (TMR) containing hydrogenated palm oil or TMR enriched with polyunsaturated fatty acids, fermented with *L. bulgaricus* S06, S04 or S09. The models, classifying samples according to feeding type and probiotic strain, achieved recognition accuracies of 97–99.5% and prediction accuracies of 97–98%. Milk fermented with *L. bulgaricus* S06 yielded 100% correct classification and exhibited distinct biochemical and volatile profiles independent of the feeding regime,

highlighting the strain's metabolic activity in the overall fermentation signature.

3. Qualitative analysis of the key wavelengths of NIRS contributing to the classification of fermented milk from cows fed either a Total Mixed Ration (TMR) containing hydrogenated palm oil or TMR enriched with polyunsaturated fatty acids, fermented with *L. bulgaricus* S06, S04, or S09, revealed that the most significant features were concentrated in the 1600–1800 nm range. Peaks at 1642, 1680, 1712, and 1726 nm, corresponding to C–H and C=O vibrational overtones, reflect bonds typical of saturated and unsaturated fatty acids, respectively. The consistent spectral patterns in this region across all strains indicate that fatty acid composition, particularly the double bonds of unsaturated fatty acids, serves as a robust, strain-independent marker for characterizing milk from different feeding regimes. Similarly, the 1300–1600 nm region, dominated by O–H overtone absorption, reflects water structure and its interactions with proteins and carbohydrates, driven by strain-specific metabolic activity.

4. The odour fingerprint of control and experimental fermented milk samples (fermented with *L. bulgaricus* S06*,*

S04 or S09) obtained from cows fed with Total Mixed Ration (TMR) containing hydrogenated palm oil or TMR enriched with polyunsaturated fatty acids, respectively, revealed higher levels of 1-hexen-3-one, 1 hexen-3-ol, hexanal, and (Z)-4-heptenal in the experimental groups. These volatiles, products of unsaturated fatty acid oxidation, played a key role in differentiating strains. The e-nose showed strong sensitivity to these aroma compounds, effectively distinguishing samples based on fermentation and feed-induced aroma differences.

5. NIRS based principal component analysis–linear discriminant analysis (PCA-LDA) models for classifying Trappista cheeses produced from milk of cows fed either a Total Mixed Ration (TMR) containing hydrogenated palm oil or TMR enriched with polyunsaturated fatty acids, and aged for 4, 8, or 12 weeks under control storage, achieved 100% recognition and prediction accuracy. This highlights the model's effectiveness in detecting feed-induced molecular and age-dependent (ripening) changes in the respective cheeses. Specific spectral markers evolved: at 4 weeks, unsaturated fatty acids (1712, 1726 nm) and water (1450 nm) dominated; by 8 weeks, protein (1500 nm) and saturated fats (1771 nm) became more prominent; and at 12 weeks,

saturated fats (1770 nm) prevailed, with reduced signals from unsaturated fats due to oxidation.

LIST OF PUBLICATIONS IN THE FIELD OF STUDIES

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Majadi, M., Barkó, A., Varga-Tóth, A., Suleimenova Maukenovna, Z., Dossimova, Z. B., Senkebayeva, D., Lukacs, M., Kaszab, T., Mednyánszky, Z., & Kovacs, Z. (2024). Quality assessment of reconstituted cow, camel and mare milk powders by near-infrared spectroscopy and chemometrics. Molecules, 29. https://doi.org/10.3390/molecules29173989

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Kovacs, Z., Lukacs, M., Bazar, G., Gillay, Z., Bosquez, Aguinaga, JP., Majadi, M., Vitalis, F. (2025). Recent results of near infrared spectroscopy on the way “from farm to fork” or even further. In K. Bec & C. Huck (Eds.), Proceedings of the 21st International Conference on Near Infrared

Spectroscopy. ICNIR 2023. Springer. https://doi.org/10.1007/978-3-031-84794-3_10

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