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**Application of ATR-FTIR Incorporated with Multivariate Data Analysis for Discrimination and Quantification of Urea as an Adulterant in UHT Milk**

(2023) *Foods*, 12 (15), art. no. 2855, .

DOI: 10.3390/foods12152855

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**Abstract**

Urea is naturally present in milk, yet urea is added intentionally to increase milk's nitrogen content and shelf life. In this study, a total of 50 Ultra heat treatment (UHT) milk samples were spiked with known urea concentrations (0–5 w/v%). Attenuated total reflectance–Fourier transform infrared (ATR-FTIR) spectroscopy with principal component analysis (PCA), discriminant analysis (DA), and multiple linear regression (MLR) were used for the discrimination and quantification of urea. The PCA was built using 387 variables with higher FL > 0.75 from the first PCA with cumulative variability (90.036%). Subsequently, the DA model was built using the same variables from PCA and demonstrated the good distinction between unadulterated and adulterated milk, with a correct classification rate of 98% for cross-validation. The MLR model used 48 variables with p-value < 0.05 from the DA model and gave R<sup>2</sup> values greater than 0.90, with RMSE and MSE below 1 for cross-validation and prediction. The DA and MLR models were then validated externally using a test dataset, which shows 100% correct classification, and the t-test result (p > 0.05) indicated that the MLR could determine the percentage of urea in UHT milk within the permission limit (70 mg/mL). In short, the wavenumbers 1626.63, 1601.98, and 1585.5534 cm<sup>-1</sup> are suitable as fingerprint regions for detecting urea in UHT milk. © 2023 by the authors.

**Author Keywords**

adulterants; discriminant; Fourier transform–infrared spectroscopy; milk fraud; regression analysis; urea

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**Publisher:** Multidisciplinary Digital Publishing Institute (MDPI)

**ISSN:** 23048158

**Language of Original Document:** English

**Abbreviated Source Title:** Foods

2-s2.0-85167563752

**Document Type:** Article

**Publication Stage:** Final

**Source:** Scopus

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