M83 Detection of adulteration in milk using infrared spectroscopy and machine learning. H. Asseis Neto[1,3], W. L. F. Tavares[2], D. C. S. Z. Ribeiro[2], J. S. Lima[2], S. V. A. Campos[3], and L. M. Fonseca*[2], [1]*Instituto Federal de Mato Grosso do Suo, Três Lagoas, MS, Brazil,* [2]*Veterinary School, Universidade Federal de Minas Gerais, Belo Horizonte, MG, Brazil,* [3]*Department of Computer Science, Universidade Federal de Minas Gerais, Belo Horizonte, MG, Brazil.*

Milk is one of the most important foods of humankind, and its production and commercialization in the industry require constant monitoring of its nutritional quality. Brazilian official laboratories monitor the quality of milk with analyzes that measure the composition and the microbiological quality. One of the concerns is the detection of frauds with the presence of any type of adulterants, a common illegal practice in Brazil and other countries worldwide. Among the analyses performed by the laboratory, some use Fourier transform infrared spectroscopy (FTIR) equipment. These methods generate a huge amount of data, which can be explored by computational techniques. The purpose of this work was to create a computational tool using data mining and machine learning techniques that characterize samples of infrared milk spectra to identify common adulterations in milk. More than 10 thousand samples, including 2376 were adulterated with foreign substances, which generated data from the infrared spectrum of the different milk samples. The obtained data were used to train machine learning models that could classify new and unknown milk samples as pure or adulterated. Neural network and decision tree models were trained with the spectral data from the FTIR readings and the classification task was performed considering binary and multiclass problems. In binary classification, the goal was to assert the presence or absence of an adulterant, while in the multiclass classification the specific adulterant classes were considered. The metrics obtained from each execution were classification accuracy and F1 score. The neural networks offered better results in general cases, with classification accuracies rates 84.65% to 97.16%. The carried out experiments showed the viability of the application of machine learning models for the detection of milk adulteration with the classification of samples. Training models with known sample data and their tests with different data sets provide a realistic view of the quality of the models, so one can confirm the ability of the model to classify instances correctly when submitted to unknown data sets.

Key Words: milk adulterants, Fourier transform infrared (FTIR), machine learning

M84 Oxidation kinetics of bioactive milk lipids using differential scanning calorimetry. S. Cheng*, L. Wei, K. Muthukumarappan, and S. Martinez-Monteagudo, *South Dakota State University, Brookings, SD.*

The consumption of certain fatty acids naturally found in milk has been associated with several health benefits. These fatty acids are known as bioactive lipids (BML), and they provide beneficial effects beyond their basic nutrition. Examples of such fatty acids are conjugated linoleic acid (CLA, C18:2), *trans*-vaccenic acid (TVA, C18:1 t11), eicosapentaenoic acid (EPA, C20:5 ω3), and docosahexaenoic acid (DHA, C22:6 ω3). Dairy processors are actively exploring ways to incorporate BML in their formulations via fortification and enrichment protocols. Chemically, BML are unsaturated fatty acids containing at least one double bond in their structure, which makes them more prone to oxidation than the saturated fatty acids. In this work, the oxidation kinetics of DHA, EPA, CLA, and TVA was studied using differential scanning calorimetry (DSC) under different heating rates (3, 6, 9, 12, 15 and 18°C min^{-1}) in the temperature range of 50–300°C. The Kissinger-Akahira-Sunose (KAS) method was used to evaluate the kinetic triplet [activation energy, E_a; pre-exponential factor, A; and reaction model, $f(\alpha)$]. The E_a values were 59.30 ± 4.75, 47.17 ± 3.15, 55.46 ± 2.75, and 57.43 ± 3.01 kJ mol^{-1} for DHA, EPA, CLA, and TVA. The isoconversional analysis revealed that the E_a values does not vary with the degree of oxidation, indicating that the oxidation of BML can be explained by a single-step approach. Several reaction models were tested, and it was found that BML follow a first-order reaction. The calculated kinetic triplets are used to predict the oxidation, and the simulated data agreed well (R^2 = 0.998) with the experimental data. The use of isoconversional methods opens up opportunities in exploring the oxidation of milk fat and it offers advantages over the traditional kinetic methods.

Key Words: bioactive milk lipid, differential scanning calorimetry, oxidation

M85 Use of infrared spectroscopy to estimate the lactose content in hydrolyzed milk. D. C. S. Z. Ribeiro[1], W. L. F. Tavares[1], J. S. Lima[1], H. Asseiss Neto[2,3], S. V. A. Campos[3], and L. M. Fonseca*[1], [1]*Veterinary School, Federal University of Minas Gerais, Belo Horizonte, MG, Brazil,* [2]*Federal Institute of Mato Grosso do Sul, Três Lagoas, MS, Brazil,* [3]*Department of Computer Science, Federal University of Minas Gerais, Belo Horizonte, MG, Brazil.*

Lactose is the main carbohydrate in milk, accounting for around 5% of its composition. It is estimated that more than half of the world population suffers from lactose maldigestion, which is the inability to digest lactose due to low production or absence of the intestinal enzyme lactase (FAO, 2013). This enzyme allows the breakdown of the lactose into glucose and galactose that will be absorbed by the intestine. Lactose accumulation in the intestinal lumen leads to fermentation by the microbiota, causing discomfort such as bloating, colic and diarrhea. Enzymatic hydrolysis, through the action of the β-galactosidase, is an efficient method to reduce the lactose content in milk and dairy products. The objective of this work was to investigate the methodology of Fourier-transform infrared spectroscopy (FTIR) to estimate residual lactose in milk. A total of 33 samples of raw milk, 20 samples of hydrolyzed milk, 52 fortified samples with 4 sugars (lactose, glucose, galactose, sucrose) were used in concentrations of 0.1; 0.5; 1.0 and 5.0%. Composition, freezing point (FP) and somatic cell count (SCC) analyses were performed. The results were provided in spreadsheets with the compositional values, FP, SCC and it were observed that lactose readings by FTIR suffer interference from the other sugars. Even hydrolyzed milk, ie lactose-free, shows a reading within the normal parameters in the lactose column. The results showed that the lactose reading by FTIR is influenced by different sugars present in the milk due to the PLS curve pre-established in the equipment, considering the same absorbance points in the infrared spectrum. The spectral data were used for the application of data mining techniques and machine learning, creating models of decision trees and artificial neural networks (ANN). The region of the spectrum that determines the sugars appears to comprise the range of 875 to 1481cm^{-1}. Preliminary data obtained by data mining of the spectra has indicated the possibility of distinguishing the different sugars present in the milk.

Key Words: residual lactose, Fourier transform infrared (FTIR), machine learning

M86 Machine learning applied to Fourier-transform infrared spectroscopy for detection of cheese whey addition to raw milk. J. S. Lima[1], D. C. S. Z. Ribeiro[1], W. L. F. Tavares[1], H. Asseiss Neto[2,3], S. V. A. Campos[3], and L. M. Fonseca*[1], [1]*Veterinary School, Universidade Federal de Minas Gerais, Belo Horizonte, MG, Brazil,* [2]*Instituto Federal do Mato Grosso do Sul, Três Lagoas, MS, Brazil,* [3]*Department*