## ESSENTIAL MINERALS, TOTAL POLYPHENOLS, NIR SPECTROSCOPY, AND RGB: AN EVALUATION OF TRADITIONAL INFUSIONS BY DATA FUSION COMBINED WITH CHEMOMETRICS

Michel Rocha Baqueta<sup>a</sup>, Grasieli Beloni de Melo<sup>a</sup>, Elem Tamirys dos Santos Caramês<sup>a</sup>, Patrícia Valderrama<sup>b</sup>, Juliana Azevedo Lima Pallone<sup>c</sup>

## **Abstract**

**Introduction:** The hot infusions of mate tea (*Ilex paraguariensis*), star anise (*Illicium verum* Hook. f.), and coffee (Coffea arabica/C. canephora) are globally consumed and appreciated by many consumers in different countries. In the scientific literature, both of them have already proven to be sources of bioactive and nutritional compounds, in addition to exhibiting stimulant and nutraceutical benefits. At the same time, the area of food analytical methods needs green techniques as vibrational spectroscopy and smartphone image to further explore the properties of the foods and beverages. Objectives: This study demonstrates the applicability of an innovative approach based on low-level data fusion combined with other chemometrics tools for evaluating mate tea, coffees (traditional, espresso and instant), star anise and their infusions to trace patterns of similarity between them. Materials and methods: Seven essential minerals (calcium-Ca, magnesium-Mg, iron-Fe, zinc-Zn, potassium-K, copper-Cu, and manganese-Mn) and total phenolic content (TPC) were determined in the solid and infusion samples. Moreover, near-infrared (NIR) spectra and RGB (red, green and blue) intensities provided by a smartphone were acquired in both samples. Then individual data sets were concatenated by a low-level data fusion approach. After data fusion, the results were evaluated with principal component analysis (PCA). **Results and Discussion**: The TPC and mineral concentrations were lower for infusions than for solid fractions, but a high leachability was assessed in the samples for TPC, Ca, Mg and K. NIR spectra and smartphone image reinforced these distinctions. The analytical data fusion approach coupled with PCA was adequate for assessment of traditional infusions with different sources. In general, solid fractions were discriminated from their respective infusions on first PCA dimension, while the second PCA dimension discriminated the samples showing the relation between them, making possible verify similarities between samples coming from different systems according type of matrix: solid or infusion. The solid samples from star anise and traditional coffee presented a similarity with infusion samples from star anise, instant, espresso, and traditional coffees, associated with Ca, Fe, Cu, and Mn levels. These results suggest that even with differences on the matrix sources, there is a similar behavior between them (solid and liquid fractions) associated with mineral content. Conclusions: Our low-level data fusion approach combined with PCA showed promising results and the possibility to use it to simultaneously evaluate complex foods coming from different systems in future studies.

**Keywords:** Data fusion approach, Infrared and image techniques, Multivariate analysis, Simultaneous analysis, Alcohol-free beverages.

<sup>a</sup> PhD Students in Food Science at University of Campinas – UNICAMP, Faculty of Food Engineering, Department of Food Science, Campinas, São Paulo, Brazil. michelbaqueta@gmail.com; grasibeloni@gmail.com; elem.carames@gmail.com; <sup>b</sup> Professor at Universidade Tecnológica Federal do Paraná – UTFPR, Campo Mourão, Paraná, Brazil. pativalderrama@gmail.com; <sup>c</sup> Professor at University of Campinas – UNICAMP, Faculty of Food Engineering, Department of Food Science, Campinas, São Paulo, Brazil. jpallone@unicamp.br