Data Article

Data on roasted coffee with specific defects analyzed by infrared-photoacoustic spectroscopy and chemometrics

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ABSTRACT

This article contains data related to the research article entitled "Quantitative assessment of specific defects in roasted ground coffee via infrared-photoacoustic spectroscopy" (Dias et al., 2018) [1]. A method potentially able for assessing the quality of roasted ground coffees is described in the origin paper. Infrared spectroscopy and photoacoustic detection (FTIR-PAS) associated with multivariate calibration were used. The samples were obtained blending whole and healthy coffee beans (*C. arabica* and *C. canephora*) with specific blends of defects, named *selections*, which contain broken, sour, and black beans, skin, woods and healthy beans still not collected. In addition to a reduction in commercial value, the presence of defects compromises the sensory attributes of coffee. On the other hand, selections are commonly found in

coffee crops and can be added intentionally to the product. Twenty-five selections were used to obtain a panel of 154 blends. The FTIR-PAS spectra of each sample generated the prediction model of Partial Least Squares Regression parameters, which are also presented here.

Specifications Table

Subject area	Agricultural science
More specific subject area	Food chemistry
Type of data	Table, figure/graph
How data was acquired	Trained coffee selectors from Instituto Agronômico do Paraná – IAPAR – Brazil classified the selections (mixtures of healthy coffee beans and defects of coffee). Samples spectra were acquired using a Bruker FTIR spectrometer (Billerica, USA) - Tensor 37, coupled to a Gasera photoacoustic detector (Turku, Finland) - PA 301, interfaced with a DSP Module. Data were processed with MATLAB R2007 / PLS Toolbox 5.2 from Eigenvector Research.
Data format	Raw and analyzed.
Experimental factors	The raw coffee material were supplied by IAPAR. Samples of healthy beans of *Coffea arabica* (Arabica) and *Coffea canephora* (Robusta), namely *bases*, in three different proportions (0%, 20% and 50% of Robusta), and 25 blends of defective and healthy beans of Arabica, namely *selections*, were explored. Then, samples were obtained blending the bases with two levels of each selection (20% and 40%).
Experimental features	One hundred and fifty-four FTIR-PAS spectra (each spectrum is an average of three replicates, numbering 462 acquisitions) and their intensity values at 1763 wavelength values were organized as a 154 $\times$ 1763 matrix. PCA (Principal Component Analysis) and PLS-DA (Partial Least Squares with Discriminant Analysis) were then performed.
Data source location	The healthy coffee beans and selections were harvested/collected in Londrina – Paraná – Brazil: Latitude -23.29, Longitude -51.17; 23° 17′ 34′′ S, 51° 10' 24′′ W, humid subtropical climate.
Data accessibility	With this article
Related research article	Dias et al. [1]

Value of the data

- Data would be available as reference to agricultural and food science, notably for coffee quality researches.
- Representative coffee material based on real situations of harvesting were explored. These *selections* composed the samples also described herein. We are not aware of the occurrence of such information in the literature.
- The presented chemometric results are an interesting material for studies on multivariate statistical analysis.
- Data on chemometrics applied for FTIR-PAS spectra of roasted ground coffee with several levels of quality can be useful for future studies of coffee quality monitoring. Thus, this investigation is particularly interesting to regulatory and supervisory agencies.