PC22. ATR-FTIR Spectroscopy for determination of free acidity, electrical conductivity, ash and total polyphenol content in honey.

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The attenuated total reflectance Fourier transform infrared spectroscopy (ATR-FTIR) could be used for food analysis determinations and food quality monitoring. This technique presents advantage because doesn't need an extensive sample preparation.

Several honey parameters are defined in standards and need to be measured in order to evaluate the honey quality.

Different commercial honeys from Portugal and Spain, with different floral sources were used in this study. All honey samples were tested for ash content, free acidity and electrical conductivity. All determinations were done using methods adopted by the International Honey Commission. Total phenol content was determined by a modification of the Folin–Ciocalteau method and the results expressed as mg of gallic acid equivalents (GAE)/100 g of honey. A total of 50 honey samples were measured

This study compares the results of Fourier transform infrared spectroscopy using an attenuated total reflection window (ATR-FTIR) with the physico-chemical parameters for different honey samples analyzed by reference methods.

ATR - FTIR spectra were acquired with a Bruker FT-IR spectrometer (Alpha) using a diamond single reflection attenuated total reflectance (ATR) device and a zero filling of 2. Duplicate spectra per sample were obtained with 32 scans per spectrum at a spectral resolution of 4 cm^{-1} in the wavenumber range from 4000 to 400 cm^{-1}. Principal component analyses (PCA) and partial least squares regression (PLS-R) modeling were performed using OPUS Quant 2 (Bruker Optics, Ettlingen, Germany).

The mean values and standard deviation for analyzed parameters were: electrical conductivity – 451(mS/cm) ± 287,4; ash content – 0,18 % ± 0,17; Free acidity – 28,3 meq/kg ± 9,3; Total phenols content – 36,20 mg GAE/100g ± 23,9; which covers a high variability and gives consequently a better calibration model.

PLS-R modeling could be a good methodology to predict ash content, free acidity, electrical conductivity and total phenol content in honey samples (Table 1), with the advantage of ease of operation, speed, no sample pre-treatment and solvent free. Therefore, the technique is an alternative to the standard methods for routine analysis or control at-line of production processes.

Table 1 - Cross validation and validation results of the calculated models for honey samples

Parameters	Preprocess	Cross validation			Validation		
		r^2	RMSECV	RPD	r^2	RMSECV	RPD
Electrical conductivity	1st d+MSC	0.925	92.4	3.64	0.854	100	2,65
Ash content	1st d	0.970	0,028	4,02	0.934	0.036	4,02
Free acidity	Const of v	0.824	4.6	2.4	0.605	4.7	1.61
Phenols content	Min-max N	0.844	8.14	2.53	0.803	9.44	2.3

d –derivative; MSC – multiplicative scatter correction; N – normalization; Const of v – constant offset validation; RMSECV – root mean square error of cross-validation; RPD - ratio of the standard deviation of the reference values of the validation samples

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