Food Control 94 (2018) 284–288

Contents lists available at ScienceDirect

Food Control

journal homepage: www.elsevier.com/locate/foodcont

Short communication

Organic and conventional coffee differentiation by NMR spectroscopy

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ARTICLE INFO

Keywords:
Coffea arabica
Roasted coffee
Organic food
NMR spectroscopy
Metabolites

ABSTRACT

The present study reports the application of ^{1}H NMR profiling for the differentiation of organic and conventional *Coffea arabica* roasted coffee samples. NMR data of coffees with different geographical origins have been analyzed by chemometrics for a possible metabolite differentiation. Classification methods like OPLS-DA allowed to highlight fatty acids, β-(1-3)-D-galactopyranose, β-(1-4)-D-mannopyranose, quinic acid and its cyclic ester as the characteristic metabolite for organic coffee, while trigonelline, CGA isomers, caffeine and acetate for conventional ones. The use of Orthogonal Signal Correction (OSC) filters improved the samples differentiation confirming fatty acids, β-(1-3)-D-galactopyranose, quinic acid and its cyclic ester as the major metabolites characterizing organic roasted coffee, while conventional resulted enriched in trigonelline and CGA isomers. The preliminary data here presented indicated ^{1}H NMR spectroscopy as a valid method for farming differentiation of *C. arabica* roasted coffee.

1. Introduction

Coffee raised high economical values being one of the most consumed beverages worldwide. A dominant role is played by both the agronomical and environmental conditions which directly influence the final quality and the metabolic composition, especially from nutritional and toxicological prospective, whose dynamics are still not fully understood. In these last years, several studies have been published focused on the organic foods such as fruits, vegetables, dairy, and poultry production (Erich et al., 2015; Kobi et al., 2018; Llano, Muñoz-Jiménez, Jiménez-Cartagena, Londoño-Londoño, & Medina, 2018), as well as fertilization procedures (Darnaudery, Furnier & Lechaudel 2018). In an attempt to justify the premium price of organic food, several claims and arguments were used (Falguera, Aliguer, & Falguera, 2012; Fillion & Arazi, 2002) like the potential environmental benefits and the most important food safety (Garcia & Teixeira, 2017). In this respect, organic agriculture has been shown to be more energy efficient (Smith, Williams, & Pearce, 2015) when compared to the conventional one and produces less N_2O on a pre area basis. In addition, organic agriculture tends to reduce soil loss, increase soil organic matter, water holding capacity and improve the soil microbial community (Gomiero, Pimentel, & Paoletti, 2011). Many of the environmental benefits associated with the organic agriculture can be attributed to farming practices that promote diversity, and to organic inputs such as complex crop rotation, green manures, intercropping, and natural pesticides. However, organic agriculture is generally 8%–25% less productive than conventional (De Ponti, Rijk, & van Ittersum, 2012). Organic agriculture highly impacted social and political thought, leading to think that organic foods are healthier than the conventional ones (Hoefkens et al., 2009). Concerning coffee, organic practices involves: (i) no use of chemical fertilizers, pesticides, herbicides, fungicides, hormones, antibiotics or growth regulators; (ii) the use of compost, farm manure, green manure, and crop rotation to maintain and improve soil fertility; (iii) a balanced pest control farm eco-system, with healthy soil management and crop diversification; (iv) control of weeds through mechanical methods; and (v) the use of good quality, clean, uncontaminated chemical-free composted materials and nursery seedlings, both off-farm and on-farm. The relatively recent EC 2009/128 directive requested European states to achieve a sustainable use of pesticides; the Sixth Environmental Action Program of the European community in the period 2002-2012 (1600/2002/EC) formed the basis for the use of this directive on the particular thematic strategy encouraging the Member States to a further reduction of usage of plant protection products, in order to minimize impacts on humans and the environment. Labelling is regulated by the EC n. 2000/13 directive, in respect to the consumer protection, and within the European boundaries, the new label has been introduced by the EC n.271/2010 regulation, to better highlight organic production system and in compliance with control rules and certification organisms. Most of the published studies about coffee farming faced the microbiological soil properties upon organic management system of cultivation (Velmourougane, 2016), suggesting in particular microbial biomass

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https://doi.org/10.1016/j.foodcont.2018.07.013
Received 7 May 2018; Received in revised form 9 July 2018; Accepted 11 July 2018
Available online 12 July 2018
0956-7135/

carbon, boron, calcium metabolic quotient acid and alkaline phosphatase as the best indicators to distinguish the two managements systems (Azevedo et al., 2017). Other authors investigated the mineral content of coffee (De Nadai Fernandes, Tagliaferro, Azevedo-Filho, & Bode, 2002; Fernandes, Santos, Lemos, Ferreira, Nogueira & Nóbrega, 2005; Melgaço Barbosa et al., 2014) only from Brasil. Finally FT-MIR-PAS was employed to detect the variations of chemical composition between organic and conventional roasted and ground *C. arabica* coffee samples only from Colombia (Gordillo-Delgado, Marín, Cortés-Hernández, Mejía-Morales, & García-Salcedo, 2012), obtaining a good discrimination by PCA analysis. Particularly, organic coffee showed a higher content in fructose, pyrazine, pyruvic and oxalic acids. New results arose from metabolomics studies also combining different analytical techniques, demonstrated the capability to differentiate organically and conventionally grown food products, like tomatoes (Marti et al., 2018), milk (Erich et al., 2015), potatoes (Pacifico et al., 2013), and oranges (Cuevas, Pereira-Caro, Moreno-Rojas, Munoz-Redondo, & Ruiz-Moreno, 2017). The aim of this study is the evaluation of the NMR based metabolic profiles of conventional and organic roasted *Coffea arabica* from different geographical origins, to highlight possible differences in the major soluble metabolites content according to the farming procedures. As a matter of fact NMR spectroscopy plays a pivotal role in the characterization of complex matrices, and it has been largely employed in metabolomic studies of foodstuffs (Consonni & Cagliani, 2010; Fotakis, Kokkotou, Zoumpoulakis, & Zervou, 2013; Hong, 2011), as well as on coffee with the aim of geographical discrimination (Consonni, Cagliani, & Cogliati, 2012; Toci et al., 2018), quality and authentication assessment (Cagliani, Pellegrino, Giugno, & Consonni, 2013; Ciampa, Renzi, Taglienti, Sequi, & Valentini, 2010; De Moura Ribeiro, Boralle, Redigolo Pezza, Pezza, & Toci, 2017). The advantage of NMR technique relies on the possibility to monitor different classes of chemical compounds, quantitatively and within the same experiment, allowing to obtain an overview of the composition of the matrix under investigation. To the best of our knowledge, this is the first report of the use of the NMR based untargeted metabolomics in the conventional-organic coffee comparison so far.

2. Material and methods

2.1. Samples

A total of 68 samples of roasted and ground *C. arabica* coffee of different geographical origin and production periods have been recruited in Italy from local markets or directly provided by producers. Among them, 42 were conventional and 26 were organic roasted coffee (see supplementary material, Table S1). All samples have been checked by producers for ochratoxin and acrylamide levels to be in agreement with the allowed law limits in order to be sold. In addition, organic coffee samples collected on the Italian market, have to be controlled and certified by an official organization (CCPB srl, www.ccpb.it) authorized by the Ministry of Agricultural, Food and Forestry Policies (MIPAAF) and labelled accordingly with a specific authorized green stamp. The samples acquired have different expiration periods, geographical origins; the roasting conditions were not informed in the labels. At least 100 mg of each sample have been dissolved in buffered deuterated water solution and after centrifugation 400 μL of the supernatant were inserted into the 5 mm NMR tube for the analysis. A capillary containing a solution with a known concentration of deuterated three-methyl sodium propionate (TSP) has been used as external standard. All samples were investigated in double.

2.2. NMR data acquisition and processing

NMR spectra have been recorded at 300 K on Bruker Advance DMX 500 spectrometer (Bruker Biospin, GmbH Rheinstetten, Karlsruhe, Germania), operating at 11.7 T and equipped with a 5 mm reverse Z gradient probe. Monodimensional spectra have been acquired with TOPSPIN 1.2 (Bruker TOSPSPIN 1.2®) employing a solvent presaturation scheme, 256 scans over 32 K of data and a spectral width of 6000 Hz. A resolution enhancement function was applied before Fourier transformation. All spectra have been phased, baseline corrected and referred to formic acid signal at 8.424 ppm. A small region around the residual water signal was removed and the spectral region of 0.15–10 ppm was split into small integrated intervals with variable dimensions (buckets), and referred to the total area value. Other experimental details have been previously published (Consonni et al., 2012).

2.3. Statistical data analysis

Multivariate statistical analysis was performed by using SIMCA-P 13.03 software (Soft Independent Modeling of Class Analogy; Umetrics, Umea Sweden). Principal Component Analysis (PCA) and two classification approaches have been used such as Partial Least Square-Discriminant Analysis (PLS-DA) and Orthogonal Projection to Latent Structures-Discriminant Analysis (OPLS-DA), performed with Unit Variance as data pretreatment. Model validation was also checked by means of random permutation test on the Y block to overcome randomness safely or over-fitting within the model. The number of latent components was determined by cross-validation technique. T2 and Distance to the Model (DModX) tests were applied to check for the presence of outliers and to evaluate the model applicability domain for all samples. The use of Orthogonal Signal Correction (OSC) filter was also investigated to remove the uncorrelated variables to response Y, from the X matrix, providing a PLS-based solution.

3. Results and discussion

The ^{1}H NMR spectra of water extracts from *C. arabica* roasted coffee is characterized by the presence of major soluble metabolites, like chlorogenic acids (caffeoyl/feruloyl-quinic acids, namely CGA), trigonelline, *N*-methyl-pyridine, and caffeine dominating the aromatic region while organic acids (acetate, citrate, lactate, malate, and quinic acid), fatty acids, sucrose and other small components were present in the aliphatic region. More details about the metabolite content and resonance assignments could be found in recent publications (Consonni et al., 2012; Wei, Furihata, Hu, Miyakawa, & Tanokura, 2011). Representative ^{1}H NMR spectra of organic and conventional roasted coffee are shown in Fig. 1. At the first sight the two spectra appeared extremely similar; to evaluate possible differences in the metabolite content, the NMR data needed to be analyzed by chemometrics. Initially PCA was performed to highlight possible natural grouping of samples according to the farming procedures. Unfortunately by scoring the first two PC's, accounting for 42.2% of the total samples variability, it was not feasible to highlight possible markers for samples discrimination (Fig. S1), suggesting the use of supervised methods. PLS-DA was therefore performed to enhance samples separation according to the farming procedures. The PLS-DA model (Fig. S2A) resulted with three latent components endowed with good predictive capability (R^2X = 45.1%, R^2Y = 75.3% and Q^2 = 53.6%) and not generated by the casualty, as confirmed by 200 cycles of random permutation of Y variables (permutation test) showed in Fig. S2B. The corresponding score plot (Fig. S2A) obtained by scoring the first two latent components, allowed a reasonably clear separation of samples. The use of OPLS-DA, by removing the structured noise affecting data matrix, is expected to improve the class separation as well as to highlight the metabolites responsible for samples separation. The corresponding score plot (resulted in one predictive and two orthogonal components) is represented in Fig. 2A, showing a very effective separation between organic and conventional coffee with good predictive capability (R^2X = 45.1%, R^2Y = 75.3% and Q^2 = 61.3%). The inspection of the S-line plot (Fig. 2B), highlighted metabolites responsible for sample

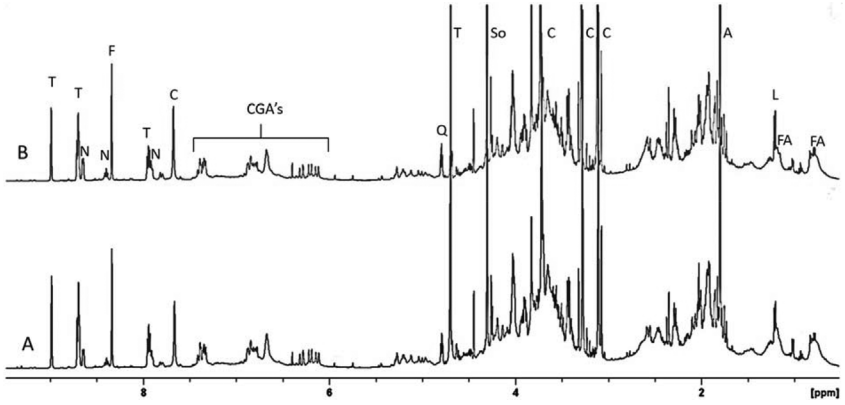

Fig. 1. [1]H NMR spectra of conventional (A) and organic (B) water extracts of *C. arabica* roasted coffee from America. Symbols as following: T, Trigonelline; N, *N*-MePyridine; F, Formiate; C, Caffeine; CGA's, Feruloyl/Caffeoyl quinic acids; Q, Quinic acid; So, residual Solvent; A, Acetate; L, Lactate; FA, Fatty Acids.

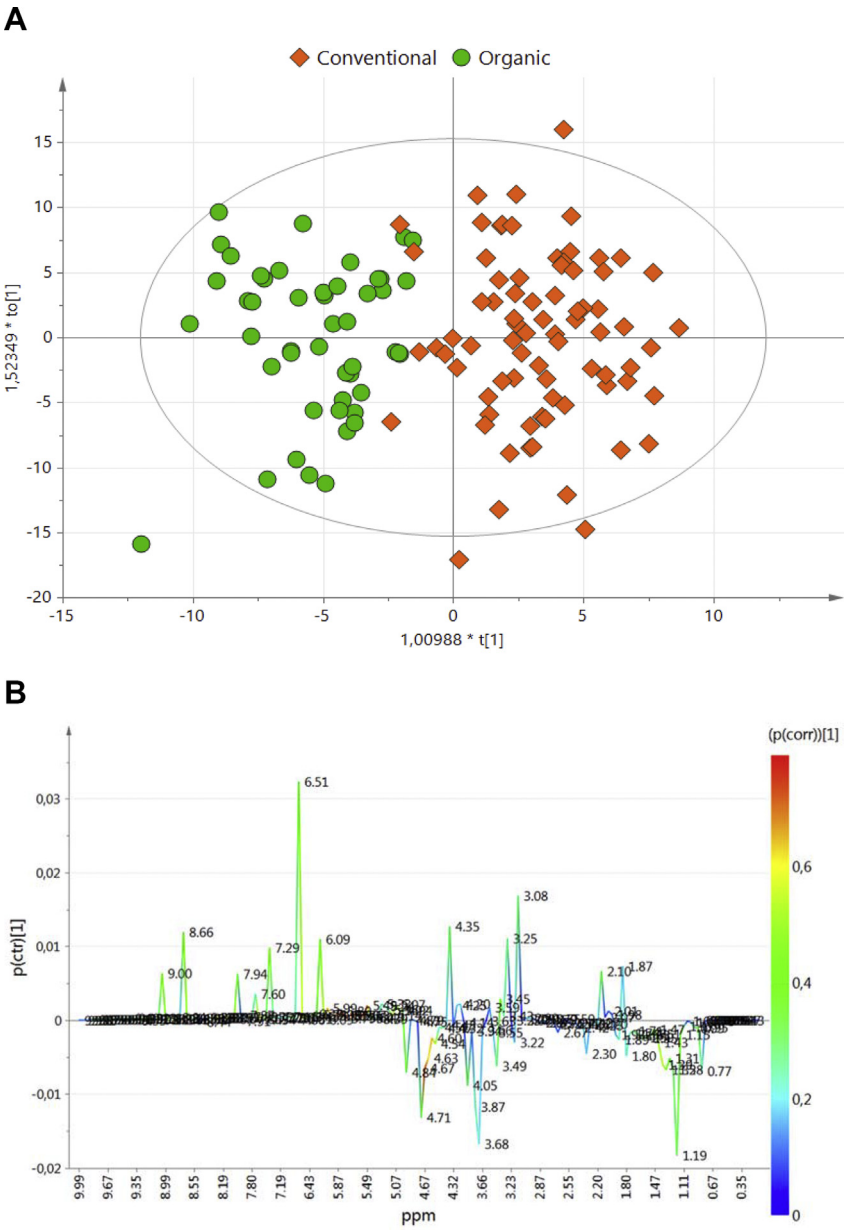

Fig. 2. (A) Score plot of OPLS-DA model of organic (green dots) and conventional (orange diamonds) roasted coffee samples. The model resulted in one predictive (12.3%) and two orthogonal components (19.8% and 13.0%). (B) S-line plot of the OPLS-DA model; p(ctr)1 loading is colored according to the absolute value of the correlation loading p(corr)1. (For interpretation of the references to color in this figure legend, the reader is referred to the Web version of this article.)

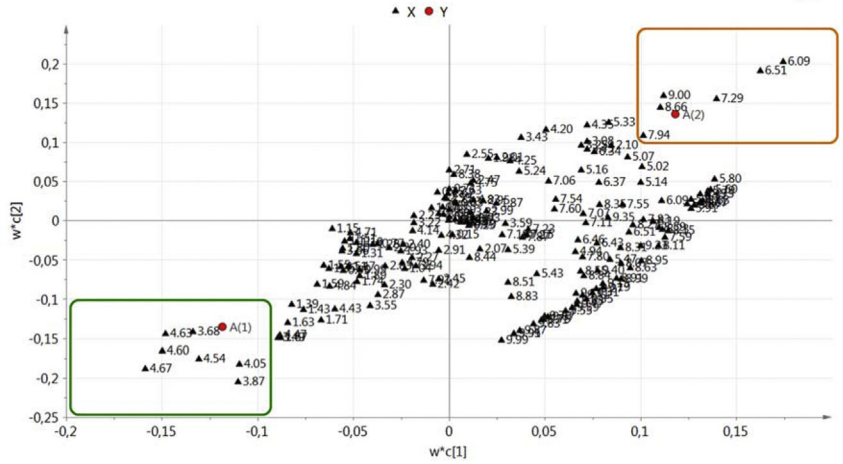

Fig. 3. Loading plot of PLS-DA model obtained with the application of two OSC filters on organic and conventional roasted coffee samples. Cutoff values of |0.1| for both w*c have been selected highlighting the variables characteristic for organic (green frame) and conventional (orange frame) roasted coffee samples. (For interpretation of the references to color in this figure legend, the reader is referred to the Web version of this article.)

differentiation. In particular, those variables close to dummy Y are endowed with the highest discriminatory power between the two classes. From this plot, organic roasted coffee samples resulted characterized by fatty acids (buckets at 1.19, 0.77, 4.67, 4.63 and 4.60 ppm ppm) β-(1-3)-D-galactopyranose (bucket at 3.68 ppm), β-(1-4)-D-mannopyranose (bucket at 4.71, 4.67 and 3.87 ppm). Finally, bucket at 4.05 ppm contains signals of quinic acid and its cyclic ester (γ-lactone). On the other hand, conventional roasted coffee resulted characterized by trigonelline (bucket at 9.00, 8.66, 7.94, and 4.35 ppm), different CGA isomers (buckets at 7.60, 7.29, 6.51, 6.09, and 2.10 ppm), caffeine (buckets at 3.25, and 3.08 ppm), and acetate (bucket at 1.87 ppm). The use of OSC filters designed to remove undesirable systematic variation within the dataset, appeared to be highly efficient even when dealing with small perturbation (Blaise, Navratil, Emsley, & Toulhoat, 2011). In the present study, the consecutive application of two OSC filters allowed to remove about 30% and 58% of uncorrelated variables respectively from the NMR data.

The classification models (PLS-DA) obtained with 1 and 2 OSC filtered data resulted in three and two latent components with good model parameters (R^2X = 47.6%, R^2Y = 84.3% and Q^2cum = 73% and R^2X = 33.6%, R^2Y = 85.6% and Q^2cum = 80.1%, respectively). Both models have been checked for casualty by 200 cycles of random permutation of Y variables (permutation test). The score plot of the PLS-DA model after two OSC filters is represented in Fig. S3.

The inspection of the corresponding loading plot (Fig. 3) confirmed fatty acids, β-(1-3)-D-galactopyranose and quinic acid and its cyclic ester as the major affecting metabolites for organic roasted coffee, while conventional roasted coffee resulted characterized by trigonelline and CGA's.

Quinic acid is one of the most bitter tasting components in roasted coffee and its larger content in in organic coffee is most likely due to chlorogenic acids decomposition. Water soluble polysaccharides are considered responsible for the "body" of coffee, which gave the creamy effect. These compounds, typically present in the insoluble form of cellulose or glycoprotein in green coffee beans, are produced during the roasting process due to heating degradation, and they resulted characterizing the organic roasted coffee.

The role of trigonelline and quinic acid has been dissected in a relatively recent paper (Wei, Furihata, Miyakawa, & Tanokura, 2014), where the chemical composition of roasted coffee has been compared with sensory perception. In particular the bitterness and body appeared related to the content of lipid, quinide and quinic acids that are negatively correlated to the sour taste of roasted coffee, thus providing sweet taste. Conversely, trigonelline is positively correlated with sour taste.

4. Conclusion

The present study represents, to the best of our knowledge, the first investigation involving the differentiation of organic and conventional roasted coffee samples, highlighted the effectiveness of the combined use of NMR and chemometrics. As a matter of fact, the wide-range metabolic profiling performed by NMR, allowed the detection of different chemical compounds simultaneously, thus providing a detailed information about the metabolite content that is influenced by the farming processes. Multivariate statistical analysis, largely facilitated the comparison and the samples discrimination, allowing to evaluate the metabolites responsible for the differentiation. The most important result of this study, is that notwithstanding different geographical origin and most likely different roasting conditions, which are known to affect the volatile fraction of roasted coffee, the water soluble metabolite fraction is containing the information necessary to distinguish organic and conventional samples. In comparison with the previous investigations on conventional/organic discrimination, the present work investigated samples obtained from geographically different continents, with different roasting conditions, respect to samples from single nation, and with the advantage of using NMR spectroscopy, the elective technique in the structural characterization of molecules.

Conflicts of interest

The authors declare no conflict of interest.

Acknowledgments

The "Scientific Foundation A. De Marco" is acknowledged for financial support of L. R. Cagliani.

Appendix A. Supplementary data

Supplementary data related to this article can be found at https://doi.org/10.1016/j.foodcont.2018.07.013.

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