Coffee authentication by near infrared spectroscopy

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Introduction

An authentic food may be defined as one which conforms to the description provided by the producer or processor. Key aspects of this description may relate to the process history of a material, the species or variety of ingredient or indeed its geographic origin. Authenticity issues may also include considerations of fitness-for-purpose.

Commercial coffee is made from Arabica or Robusta varieties or blends of these two. Arabica is superior in quality to Robusta and therefore commands a higher price, thereby introducing the potential for fraud. Previously published methods for solving this problem have used inter-varietal differences in the unsaponifiable lipid fraction[1] and the content of a range of mineral elements[2] or volatile compounds.[3] The application of near infrared (NIR) spectroscopy to qualitative analysis of foodstuffs has been previously demonstrated.[4–7] This study describes work performed to determine the utility of NIR spectroscopy and discriminant mathematical techniques for determining the authenticity of coffee samples.

Materials and methods

Samples of pure Arabica and pure Robusta coffee beans from 27 countries were collected. Coffee blends (50% Arabica & 50% Robusta) were made in the laboratory. Ground coffees were made using a domestic coffee grinder (Moulinex, France) while lyophilised powders were made after the preparation of coffee beverage (30 g ground coffee in 180 mL hot water). Spectra were recorded in reflectance mode using an NIRSystems 6500 instrument over the 400–2498 nm wavelength range. Spectral collection and file manipulation was performed using ISI software; data analysis involved principal component analysis and factorial discriminant analysis and was performed using SAISIR (INRA, Nantes, France).

Results

Ground coffee

105 roast samples were used in this part of the work—50 Arabica roast (AR), 33 Robusta roast (RR) and 22 BR (blend roasts). These were divided into a calibration set of 52 samples (25AR, 16RR and 11BR) and a prediction set of 53 samples (25AR, 17RR and 11BR). Discriminant models were developed on the basis of three clusters, i.e. pure Arabicas, pure Robustas and blends.

Using the 400–1100 nm range, the results were poor. The best model used 12 principal components but only achieved 88.5% correct classification in the calibration set. In the prediction set, only 77.4% of samples were correctly identified. Using the range 1100–2498 nm, better results were obtained. A seven component model achieved complete discrimination of the calibration set and 83.02% correct identification (44 out of 53 samples) in the prediction set. Of the nine samples

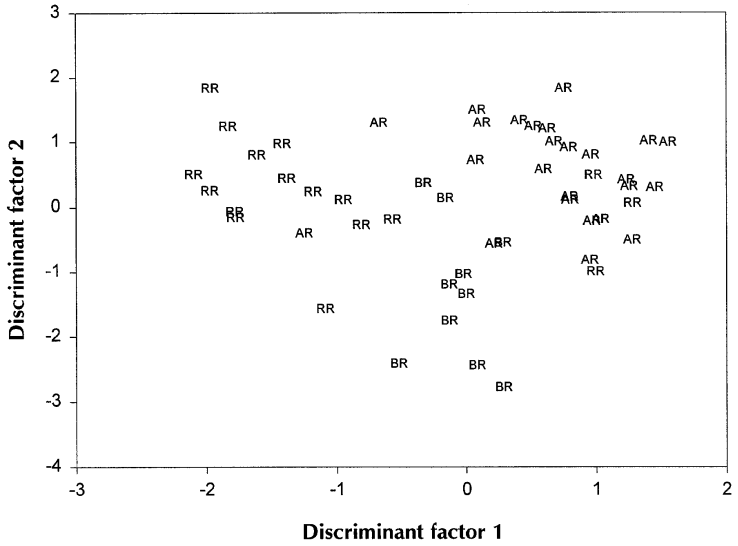

Figure 1. Discriminant score plot of prediction file—ground coffee.

mis-classified, five were mixtures. A two-dimensional representation of the spread of these samples is shown in Figure 1.

Discriminant factor 1 separates AR and RR samples while factor 2 is responsible for the separation of blends; the reason for such separation is unclear. The spectral profile of discriminant factor 1 (Figure 2) is dominated by peaks due to water (1934 nm) and oil (1722, 1760, 2306 and 2346 nm), reflecting differences in fatty acid contents of these two bean types. There may also be

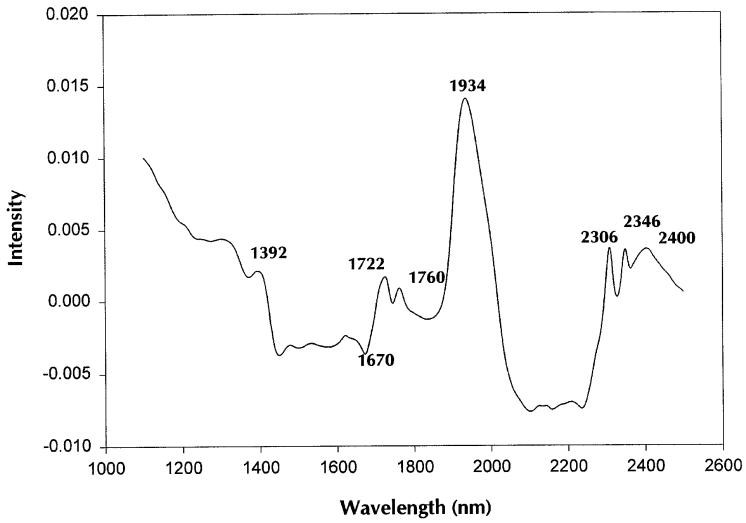

Figure 2. Discriminant profile of factor 1—ground coffee.

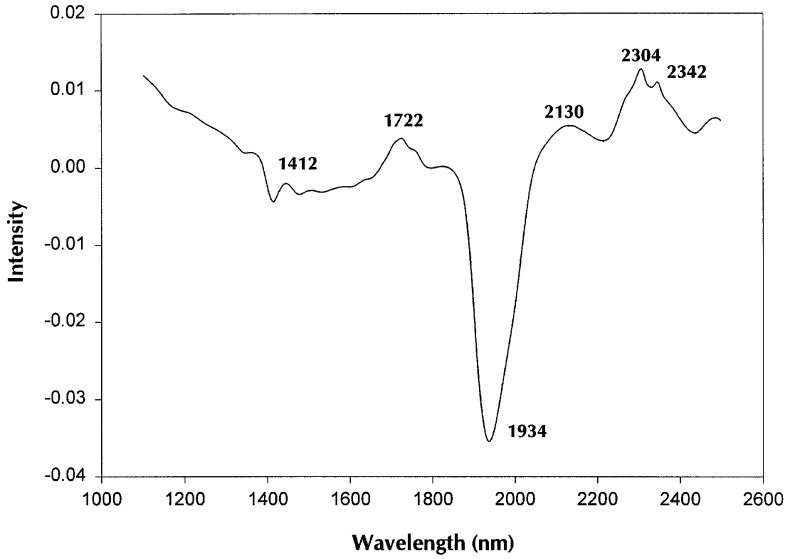

Figure 3. Discriminant profile of factor 2—ground coffee.

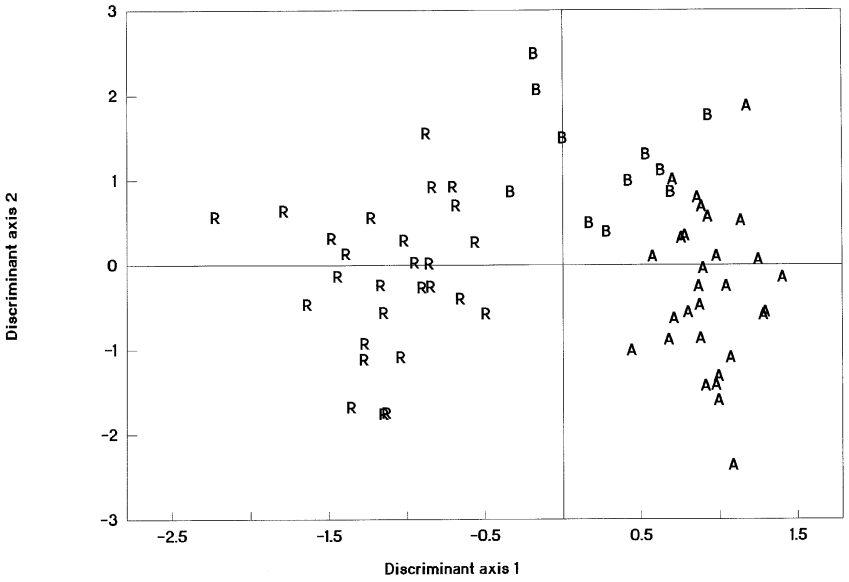

Figure 4. Discriminant scores plot of calibration sample set; lyophilised coffee samples.

a difference in mean moisture content between the two although no control over this parameter is exerted during the roasting process. Factor 2 (Figure 3) contains peaks due to water (1412 and 1934 nm) and oil (2304 and 2342 nm) in opposition to each other.

Lyophilised coffee

134 samples of coffee were used. The calibration set (67 samples) contained 27 RR, 29AR and 11 BR; the prediction set comprised 27RR, 31AR and 9BR. As was the case for the ground coffee, the 400–1100 nm wavelength range did not produce successful discriminant models.

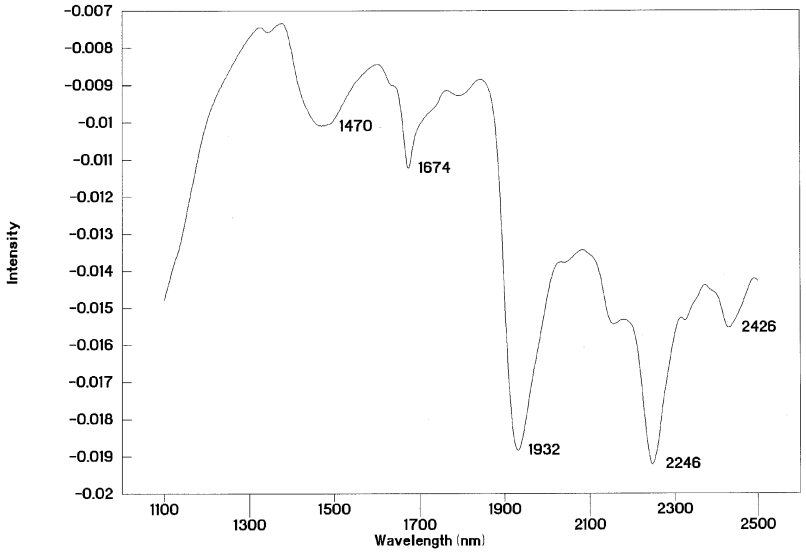

Figure 5. Profile of discriminant factor 1; lyophilised coffee samples.

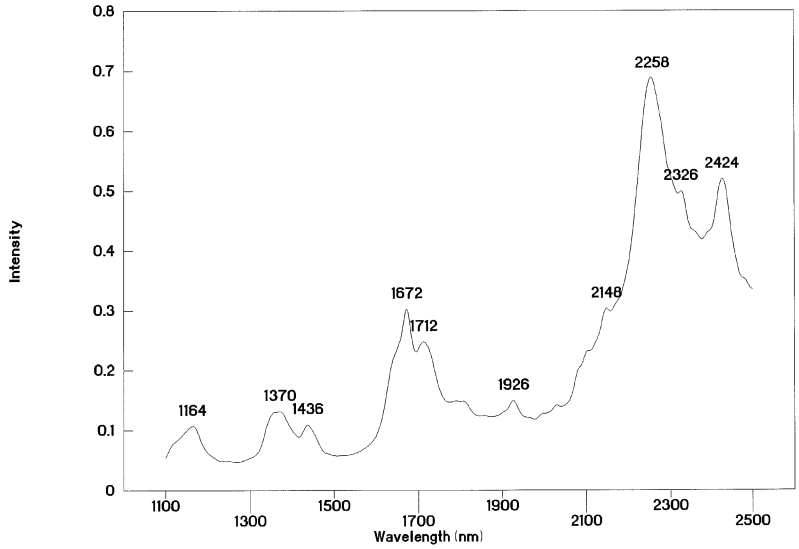

Figure 6. Reflectance spectrum of caffeine.

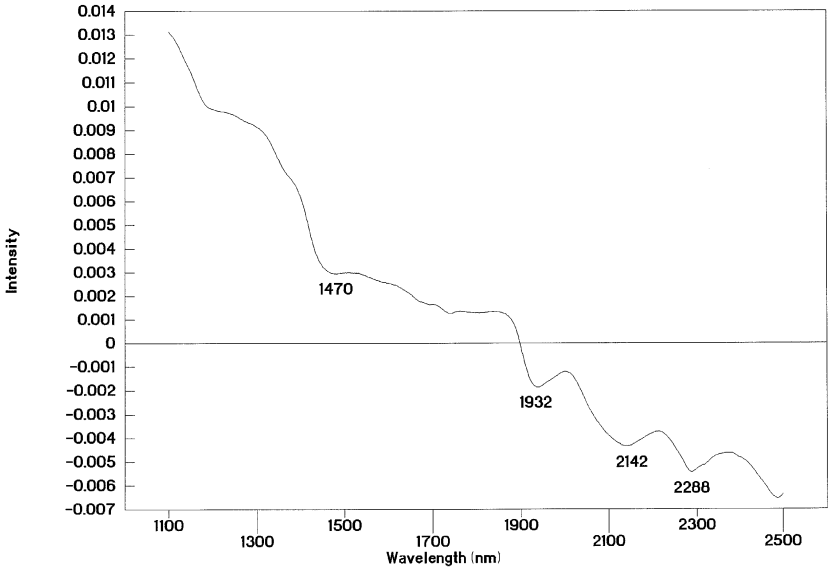

Figure 7. Profile of discriminant factor 2; lyophilised coffee samples.

Using the 1100–2498 nm wavelength range, a 12 component model achieved the maximum correct classification in the calibration set—98.51% (66 out of 67 samples). This model correctly identified 64 out of 67 samples (95.52%) in the prediction set.

The discrimination achieved in a two-dimensional plot of the calibration sample scores may be seen in Figure 4; the first discriminant factor discriminates between Arabica and Robusta varieties, while the second effects some separation between these two clusters and the blend samples.

The spectral profile of discriminant factor 1 (Figure 5) contains considerable structural detail; maxima are close to those found in caffeine (Figure 6) and this or other alkaloids may be responsible for the separation achieved. Factor 2 (Figure 7) may involve water (minima at 1470 and 1932 nm) while the trough at 2142 nm may be attributed to oil or an amide combination band. The longest wavelength feature may originate in a –CH stretch–CH deformation combination band structure, possibly from a water-soluble carbohydrate material.

Conclusions

NIR reflectance has facilitated discrimination between Arabica, Robusta and coffee blends with a high degree of success using either ground or lyophilised samples. Transfer of the technique out of the laboratory will require its extension to commercial samples, given known differences between the preparation techniques used industrially and those utilised in this work.

References

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