QA/QC of coffee using the Agilent Cary 630 ATR-FTIR analyzer

Application note

Food testing and agriculture

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Introduction

Coffee has become one of the most consumed beverages in the world due its pleasant taste and aroma. Its appeal can also in some part be attributed to its caffeine content and scientifically-reported health benefits. Its increasing popularity has inspired coffee manufacturers to produce many new and exotic blends. Coffee is prepared in multiple ways by subjecting green coffee beans to washing, boiling, drying, pressurizing, roasting and fermenting processing techniques.

Roasting is the main process in coffee preparation, and almost all coffee is roasted before it is consumed. This process influences the taste of the beverage by changing the coffee beans both physically and chemically.

During this process the coffee beans lose moisture, which decreases their weight, increases their volume, and causes a noticeable reduction in density. The density of the beans affects the product packaging requirements as well as the strength of the resulting coffee. Moreover, during roasting, caramelization can occur, because the intense heat used breaks down starches in the beans and converts them to simple sugars that begin to brown. This can change the color of the beans. The aromatic oils and acids weaken, changing the flavor, and additional oils like caffeol start to develop. The degree of roasting, therefore, has a significant effect upon coffee flavor and body. Darker roasts are generally bolder because they have less fiber content and thus a more sugary flavor. Lighter roasts are more complex and they have stronger flavors due to the presence of more original aromatic oils and acids. To minimize the effect of environmental factors like air, moisture, heat and light on the fresh coffee taste and flavor, roasted coffee beans need proper storage. Coffee is also occasionally decaffeinated and the extracted caffeine is usually sold to the pharmaceutical or the soft drink industries.

Ideally, coffee beans should be authenticated prior to their blending and packaging. A newly arrived advance sample of a bulk shipment lot (normally sent by air) may or may not be representative of the bulk material that arrives by boat or train, which can suffer temperature fluctuations leading to oxidation of lipids and the development of off flavors.

The coffee industry therefore requires an analyzer that is sensitive enough to discern both subtle and characteristic differences among commercial coffee bean commodities (Figure 1). The basic need is a quick, simple and reliable method that would allow an operator to accept or reject the coffee shipment on the spot; ideally within minutes of receiving the sample. Since coffee is a complex material, the task of quality assurance/quality control (QA/QC) is currently both time-consuming and tedious, requiring the use of internal or external chemical laboratory support. Fourier transform infrared (FTIR) spectroscopy has proven to be an ideal technique for the detection of subtle changes in the chemical composition of coffee.

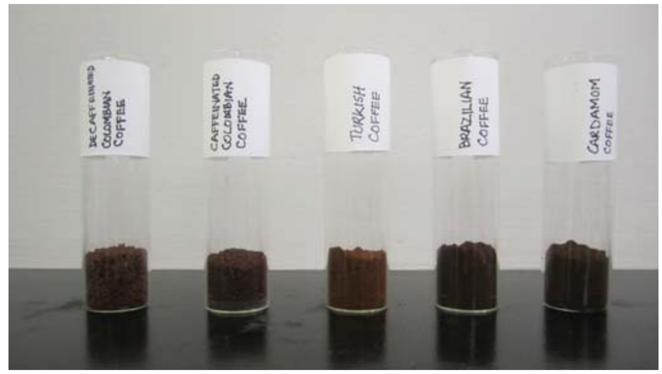

Figure 1. Various coffee powders

Experimental

1. Various commercial ground-coffee brands were purchased from several grocery stores.

2. A small amount of each ground-coffee was placed on the diamond attenuated total reflectance (ATR) crystal of the Agilent Cary 630 ATR-FTIR analyzer (Figure 2).

Figure 2. Agilent Cary 630 ATR-FTIR analyzer

3. The samples were pressed against the diamond crystal using the attached pressure clamp. A slip clutch on the clamp prevents overtightening.

4. FTIR spectra were acquired in less than 30 seconds (64 scans at 4 cm^{-1} resolution).

5. The spectra of reference (authenticated) coffee samples were automatically stored in a dedicated spectral database.

6. The spectra of new coffee lots was then analyzed using an automated output pass/fail or percentage (%) similarity.

Results and discussion

All the infrared spectra of the ground coffee samples were automatically stored in a spectral database created by using the Agilent MicroLab FTIR software. Each ground-coffee brand exhibited characteristic infrared bands between 1800 and 800 cm^{-1} (Figure 3). The 1800 to 800 cm^{-1} region contains absorbance bands attributed to the stretching vibrations of C=O groups. These bands can be ascribed to organoleptic vinyl esters, lactones, esters, aldehydes, ketones, and acids present in the brewed coffee. C-H (methylene) bending (scissoring) absorptions occur between 1470 and 1430 cm^{-1} and can be assigned to lipids, while bands appearing below 1400 cm^{-1} are referred to as the fingerprint region, as they are difficult to assign to specific functional groups. However, in this case, the strong absorptions between 1200 and 900 cm^{-1} can be assigned to C-O-H and C-O-C groups stemming from carbohydrate absorptions (for example, cellulose). The entire spectral absorption region is used to differentiate coffee samples with varying chemical compositions.

To test the capability of the Cary 630 ATR-FTIR analyzer to repeatedly record representative spectra of each coffee sample, one set of sample spectra was stored in a spectral database, and the second set was used as a series of validation samples. In all cases, the duplicate samples were correctly identified and matched. In subsequent experiments, the ATR-FTIR spectra of different sample lots were acquired and their spectra compared to those already stored in the spectral library database. In each case, the MicroLab software Search function correctly identified each coffee brand (Figure 4). In this manner, when the spectrum of a new sample is acquired, it can be compared to the reference spectra previously recorded, and the identity of the new sample can be established within seconds of spectral acquisition.

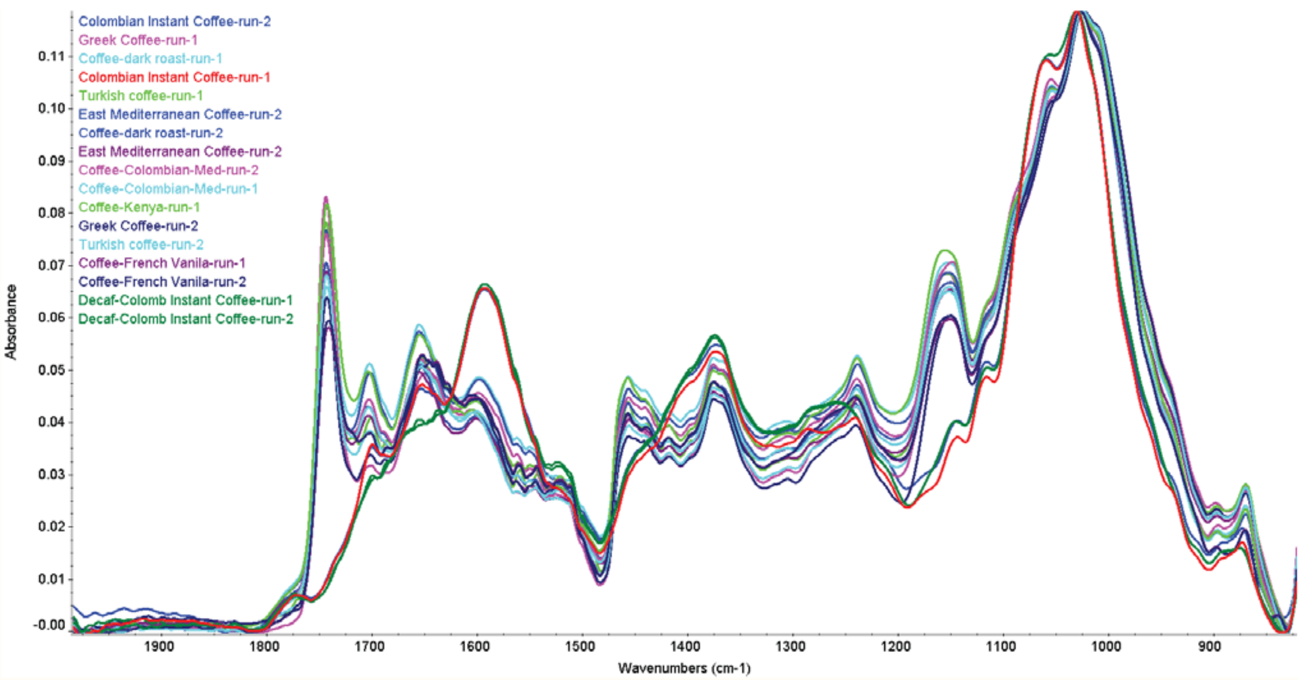

Figure 3. Infrared spectra of selected coffee powders (in duplicate)

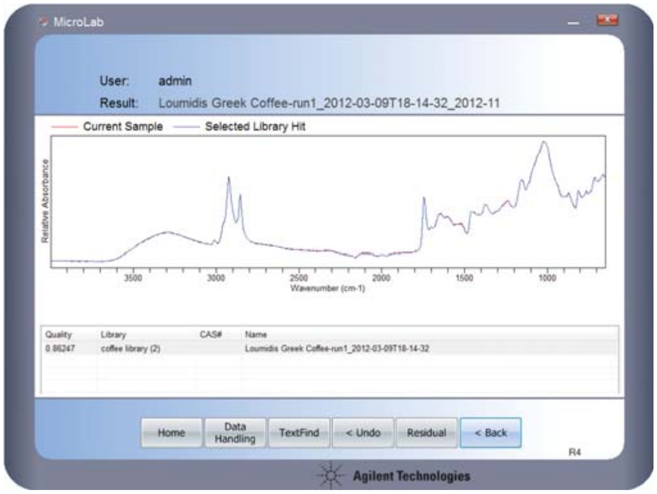

Figure 4. Correct identification of an unknown coffee sample by the Agilent MicroLab FTIR software

Conclusion

The Agilent Cary 630 ATR-FTIR analyzer is the ideal technology to detect subtle changes in the chemical composition of coffee, eliminating the need for any sample preparation or extraction procedures. The entire analysis protocol requires simply placing a small amount of sample on a diamond sampling surface, and recording the infrared spectrum. The spectral information obtained by the analyzer can be considered as the chemical fingerprint of the compound in question. A comparison of the infrared spectrum of an authenticated sample (or reference product) to that of an incoming material can establish product identity. Moreover, it is ideal for use at the receiving dock, in the process line or for onsite verification by taking it to the ingredient supplier depot.

Suggested references

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Published November 28, 2012
Publication number: 5991-0783EN

Agilent Technologies