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Application News

High Performance Liquid Chromatograph Nexera™ lite

Monitoring Content of Components with Functional Benefits in Coffee Made with Different Roasting Times

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User Benefits

- By utilizing the multi-data report function, reports for results from multiple analyses can be created quickly and efficiently.
- Human error is prevented by posting analysis results and creating graphs automatically.

■ Introduction

Coffee components with functional benefits have a variety of different physical properties and range from acidic to basic. A detailed description of simultaneous quantitative analysis of these components using a Shim-pack Scepter™ PFPP column is described in Application News No. 01-00280.

Roasting coffee beans is known to reduce the concentration of trigonelline, one of the functional components contained in coffee. It is also known that chlorogenic acid is hydrolyzed by roasting coffee beans and converted to pyrocatechol via caffeic acid and quinic acid.[1)]

This article describes some benefits of automatically transcribing changes in the content of functional components in coffee as a function of roasting time into a multi-data report.

■ Analyses of Coffee with Different Roasting Times

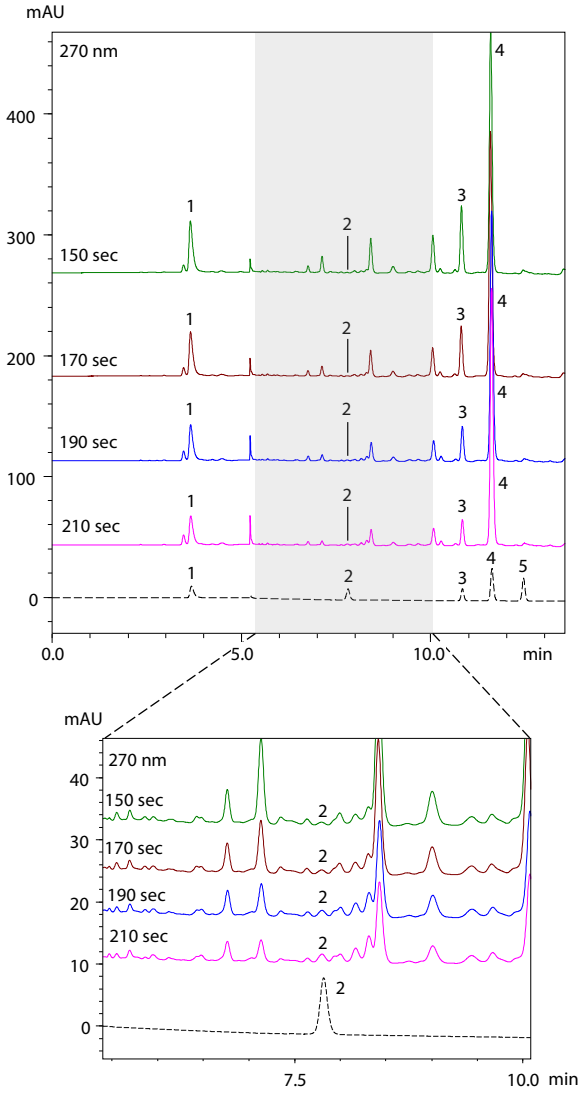
Fig. 1 shows the structural formula of trigonelline, pyrocatechol, chlorogenic acid, and caffeic acid, which were the targets of the analyses.

Samples were prepared by using 150 mL of boiling water to extract coffee from ten grams of commercial ground coffee beans with different roasting times. The samples were filtered through 0.2 µm membrane filters and diluted ten-fold with ultrapure water before HPLC analysis. The roasting times were set to four conditions at twenty-second intervals from 150 seconds to 210 seconds, with the roasting temperature set to 250 °C. Table 1 shows the analytical conditions, and Fig. 2 and 3 show the chromatograms of coffee with different roasting times.

Table 1 Analytical Conditions

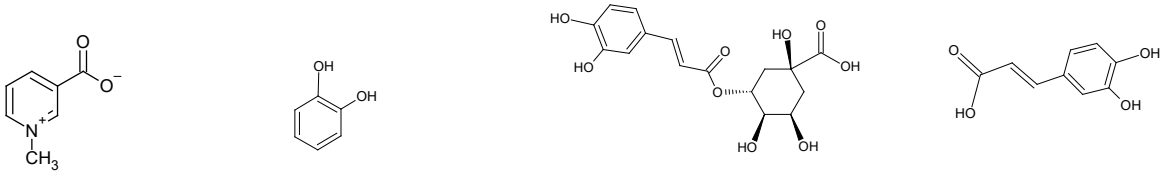
System:	Nexera lite
Column:	Shim-pack Scepter PFPP-120*1 (150 mm × 4.6 mm I.D., 3 µm)
Flowrate:	1.0 mL/min
Mobile Phases:	A) 20 mmol/L (Sodium) phosphate buffer (pH 2.6) B) Acetonitrile
Time Program:	0 % B (0.00 - 1.00 min) → 10 % B (4.00 min) → 20 % B (10.00 - 12.00 min) → 70 % B (12.01 - 13.00 min) → 0 % B (13.01 - 18.00 min)
Mixer:	180 µL
Column Temp.:	25 °C
Injection Volume:	5 µL
Vial:	SHIMADZU LabTotal™ for LC 1.5 mL, Glass*2
Detection (PDA):	Ch 1 : 270 nm; Ch 2 : 325 nm (SPD-M40)

*1 P/N: 227-31057-05 *2 P/N: 227-34001-01



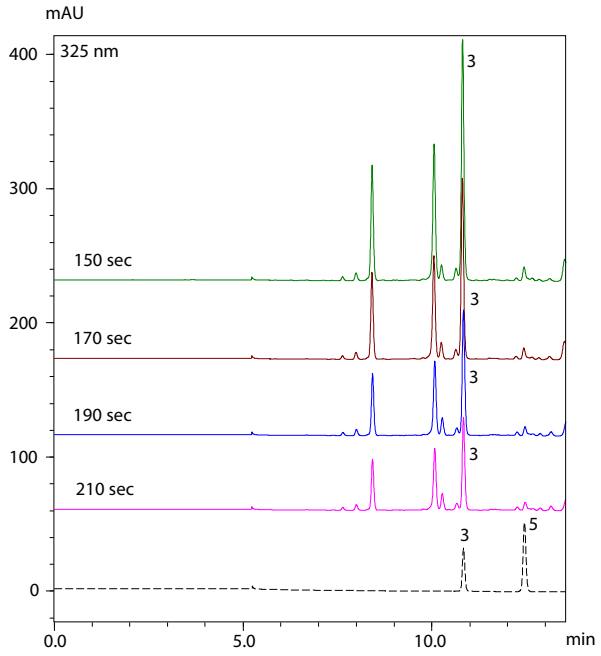
■ Peaks 1. Trigonelline, 2. Pyrocatechol, 3. Chlorogenic acid, 4. Caffeine, and 5. Caffeic acid

Fig. 2 Chromatograms of Coffee with Different Roasting Times (270 nm)
(Solid Line: Coffee; Dashed Line: Standard Solution)



Trigonelline | Pyrocatechol | Chlorogenic acid | Caffeic acid

Fig. 1 Structure of Four Target Compounds



■ Peaks 3. Chlorogenic acid, 5. Caffeic acid

Fig. 3 Chromatograms of Coffee with Different Roasting Time (325 nm)
(Solid Line: Coffee; Dashed Line: Standard Solution)

■ Calibration Curves

The calibration curves for the five target compounds were highly linear, with coefficients of determination (r^2) of 0.99999 or greater. Fig. 4 shows the calibration curves of trigonelline and pyrocatechol. Table 2 shows the concentration ranges of calibration curves and the coefficients of determination for all the target compounds.

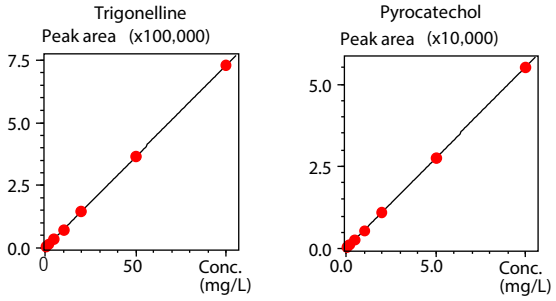


Fig. 4 Calibration Curves

Table 2 Concentration Ranges of Calibration Curves and Coefficients of Determination (r^2)

Compound	Conc. Range (mg/L)	r^2
Trigonelline	1-100	0.99999
Pyrocatechol	0.1-10	0.99999
Chlorogenic acid	1-100	0.99999
Caffeine	1-100	0.99999
Caffeic acid	0.1-10	0.99999

■ Use of Multi-Data Report Function*3

The multi-data report function is a reporting function that automatically inserts analytical results into a spreadsheet file as soon as a batch analysis is finished. The function can also be used for data post-processing to generate a report from previously acquired data. This feature eliminates the time and various risks involved in manually transcribing data, such as human errors.

In this case, the multi-data report function was used to automatically create a spreadsheet file based on the results from analyzing coffee with different roasting times (Fig. 5). As shown in Fig. 5, it is also possible to create graphs showing the concentration changes by plotting the concentration of functional components on the vertical axis with the roasting time on the horizontal axis. The graph shows that as roasting time increased, the concentrations of trigonelline and chlorogenic acid decreased and that of pyrocatechol increased. On the other hand, it also showed that the caffeine concentration was almost constant regardless of the roasting time.

*3: The multi-data report function is supported by LabSolutions™ DB/CS

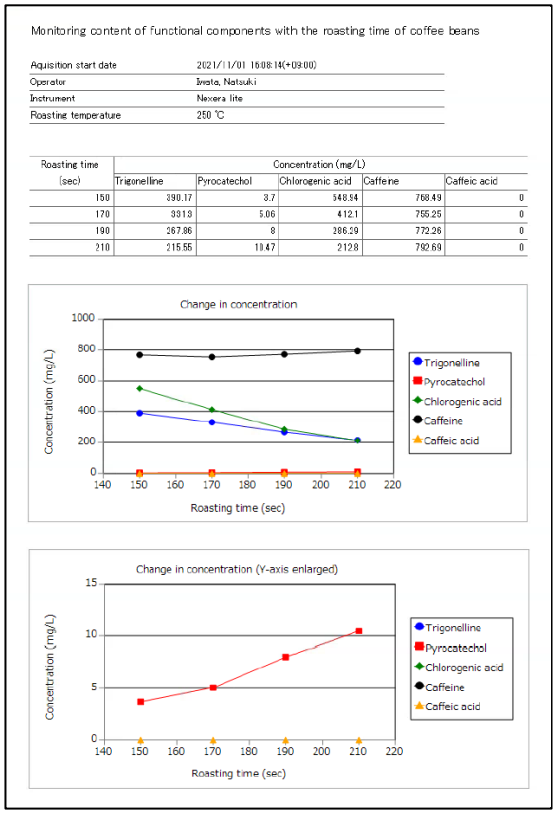


Fig. 5 Multi-Data Report Function

■ Conclusion

By utilizing the multi-data report function, it was possible to monitor the content of each functional component with respect to the roasting time of coffee using the analytical conditions developed as previously reported in Application News No. 01-00280-EN. The applications described in this article are expected to contribute to research and development in food engineering, including the study of functional components.

References

1) M. Kamiyama, J.K. Moon, H.W. Jang, T. Shibamoto, J Agric Food Chem. 63(7), 1996-2005 (2015).

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