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# An Innovative Approach to Coffee Bean Characterization, Using SEC and Principal Component Analysis

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Coffee beans are one of the largest traded commodities at international levels. Their quality traditionally has been judged by specially trained individuals who taste, smell, and visually examine the beans (sensory analysis). Although today's international trade requirements are stricter, methods for detecting trading fraud and chemical standards for characterizing coffee beans have yet to be developed. Efficient methods for characterizing coffee beans are becoming a necessity.

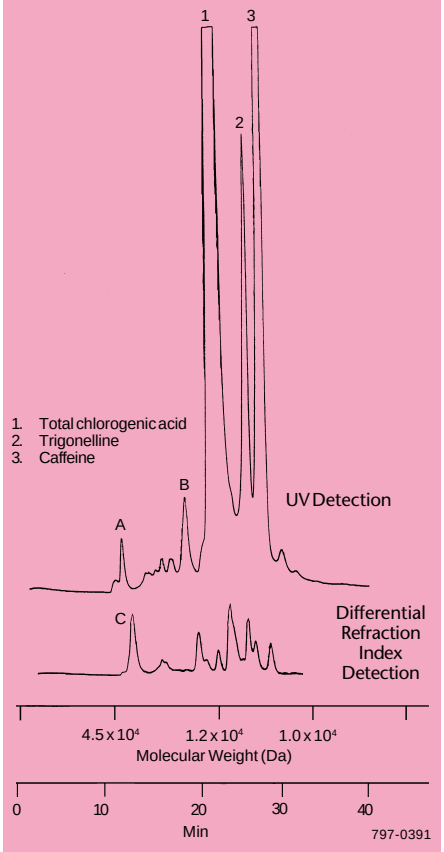
Investigators at the Universidade Federal do Rio de Janeiro, Instituto de Química characterized coffee beans by using size exclusion chromatography (SEC), with two forms of detection, and principal component analysis (PCA). SEC excludes, or fractions, compounds according to their molecular weight — molecules with larger molecular weights are eluted before those with smaller molecular weights. PCA is a statistical method that analyzes highly correlated variables using nonlinear multiple regression analysis, partial regression analysis, and least square techniques.

Six samples of green coffee beans from various countries of origin were first identified as high or low quality by sensory analysis — beans A, B, and C were of high quality; beans D, E, and F were of low quality. Each of the six samples was separated on a TSKgel G3000SW column, and analyzed with a UV detector and a differential refraction index detector. The TSKgel G3000SW column was calibrated using protein standards, to enable the investigators to split the chromatograms into several regions by molecular weight. The chromatograms in Figure A present a distinct profile showing the low and the high molecular weight regions for a low-quality bean.

The first region, up to 21 minutes, consists of molecules with larger molecular weights, greater than $1.2 \times 10^4$. The second region, 21 to 40 minutes, consists of molecules with low molecular weights, less than $1.2 \times 10^4$. This region consists of very important substances — total chlorogenic acid, trigonelline, and caffeine — shown respectively in Figure A as peaks 1, 2, and 3 (1).

**Figure A. Low-Quality Coffee Bean by SEC**

Column: **TSKgel G3000SW, 30cm x 7.5mm ID, 10µm particles**
Cat. No.: **805789**
Mobile Phase: 0.05% $N_3Na$ in twice-distilled water
Flow Rate: 0.5mL/min
Det.: UV, 0.16 AUFS, 272nm differential refraction index, 64 scale factor of 40
Inj.: 10µL of prepared sample from coffee bean D




The compounds shown as peaks A, B, and C contribute 90% of the varieties' quality attributes among the samples — their peak areas are the principal parameters representing the variability of the analyses. Therefore, these small peaks represent the final quality characteristics of coffee preparations.

Results of the chromatographic analyses were processed by a statistical method — PCA. In PCA three methods are used to assess discrimination stability: principal component analysis, modified PCA, and discriminant function analysis with cross validation. With PCA, variation of a complex system of variables can be expressed by a simple, graphical representation. System integrity and reproducibility is maintained as long as the original sample conditions are kept constant.

Results from PCA showed that SEC, particularly with UV detection, provided a remarkable separation. Furthermore, SEC is capable of simultaneous analysis of the important peaks, whereas reversed-phase HPLC requires different chromatographic conditions for each compound, and headspace-GC analysis results in a high number of crowded peaks.

Further studies are necessary to provide detailed identification of components. Additional complementary analytical techniques, such as mass spectrometry and GC or LC, can help us obtain a detailed characterization profile of most aroma and bouquet compounds for coffee.

**Ordering Information:**

| Description | Cat. No. |
|---|---|
| **TSKgel G3000SW Gel Filtration Columns**<br>30cm x 7.5mm ID, 10µm particles | **805789** |

**Reference**

1. De Maria, C. A. B., L. C. Trugo, and R. F. A. Morreira, *Food Chemistry,* **52:** 447 (1995).

Reference not available from Supelco.

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