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**When Machine Tastes Coffee: Instrumental Approach To Predict the Sensory Profile of Espresso Coffee**
Christian Lindinger, David Labbe, Philippe Pollien, Andreas Rytz, Marcel A. Juillerat, Chahan Yeretzian, and Imre Blank
**(Article), 2008**, *80* (5), 1574-1581
DOI: 10.1021/ac702196z

**Visualization of a Lost Painting by Vincent van Gogh Using Synchrotron Radiation Based X-ray Fluorescence Elemental Mapping**
Joris Dik, Koen Janssens, Geert Van Der Snickt, Luuk van der Loeff, Karen Rickers, and Marine Cotte
**(Article), 2008**, *80* (16), 6436-6442
DOI: 10.1021/ac800965g

**Water Analysis: Emerging Contaminants and Current Issues**
Susan D. Richardson
**(Review), 2007**, *79* (12), 4295-4324
DOI: 10.1021/ac070719q

**Electrochemical Sensors**
Benjamin J. Privett, Jae Ho Shin, and Mark H. Schoenfisch
**(Review), 2008**, *80* (12), 4499-4517
DOI: 10.1021/ac8007219

**Rapid Prototyping of Microfluidic Systems in Poly(dimethylsiloxane**
David C. Duffy, J. Cooper McDonald, Olivier J. A. Schueller, and George M. Whitesides
**(Article), 1998**, *70* (23), 4974-4984
DOI: 10.1021/ac980656z

**Micro Total Analysis Systems: Latest Achievements**
Jonathan West, Marco Becker, Sven Tombrink, and Andreas Manz
**(Review), 2008**, *80* (12), 4403-4419
DOI: 10.1021/ac800680j

**Cancer Cell Targeting Using Multiple Aptamers Conjugated on Nanorods**
Yu-Fen Huang, Huan-Tsung Chang, and Weihong Tan
**(Accelerated Article), 2008**, *80* (3), 567-572
DOI: 10.1021/ac702322j

**Colorimetric Method for Determination of Sugars and Related Substances**
Michel DuBois, K. A. Gilles, J. K. Hamilton, P. A. Rebers, and Fred. Smith
**(Article), 1956**, *28* (3), 350-356
DOI: 10.1021/ac60111a017

**Gold Nanoparticle-Based Colorimetric Assay for the Direct Detection of Cancerous Cells**
Colin D. Medley, Joshua E. Smith, Zhiwen Tang, Yanrong Wu, Suwussa Bamrungsap, and Weihong Tan
**(Article), 2008**, *80* (4), 1067-1072
DOI: 10.1021/ac702037y

**Fiber-Optic Chemical Sensors and Biosensors**
Otto S. Wolfbeis
**(Review), 2008**, *80* (12), 4269-4283
DOI: 10.1021/ac800473b

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JOURNAL OF AGRICULTURAL AND FOOD CHEMISTRY
ARTICLE

*J. Agric. Food Chem.* **2009**, *57*, 8705–8710 **8705**
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# Variance in the Chemical Composition of Dry Beans Determined from UV Spectral Fingerprints

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Nine varieties of dry beans representing five market classes were grown in three locations (Maryland, Michigan, and Nebraska), and subsamples were collected for each variety (row composites from each plot). Aqueous methanol extracts of ground beans were analyzed in triplicate by UV spectrophotometry. Analysis of variance−principal component analysis was used to quantify the relative variance arising from location, variety, between rows of plants, and analytical uncertainty and to test the significance of differences in the chemical composition. Statistically significant differences were observed between all three locations, between all nine varieties, and between rows for each variety. PCA score plots placed the nine varieties in four categories that corresponded with known taxonomic groupings: (1) black beans (cv. Jaguar and cv. T-39), (2) pinto beans (cv. Buster and cv. Othello), (3) small red beans (cv. Merlot), and (4) great northern (cv. Matterhorn and cv. Weihing) and navy (cv. Seahawk and cv. Vista) beans. The relative plant-to-plant variance, estimated from the between row variance, was 71−79% for 25−40 plants per row.

**KEYWORDS: Nine common beans; *Phaseolus vulgaris* L.; spectral fingerprinting; multiple locations; analysis of variance; principal component analysis; ANOVA- PCA; UV spectrometry**

## INTRODUCTION

The chemical composition of dry beans is determined by genetic, environmental, and processing factors. Some genetic factors are obvious to the consumer; pinto beans are readily distinguished from navy beans and black beans. However, the influence of the growing location, seasonal variation (e.g., rainfall, temperature, and total sun exposure), cultivation practices (organic vs conventional farming), and variation between plants can only be determined through a statistical analysis of their chemical compositions.

For nutritional purposes, the nutrient levels and variation are of primary importance. Regretfully, analysis of all of the specific vitamins and minerals can be prohibitively expensive and time-consuming, especially when large degrees of variation are experienced between plants, growing locations, and environmental conditions. Analysis of all of the specific vitamins and trace metals, however, would be time-consuming and costly. Analysis of non-nutrient but bioactive chemical components would further contribute to the cost of characterizing plant materials. A simpler approach is to compare the overall chemical composition of plant materials using spectral fingerprinting or chromatographic profiling. Thus, a single well-characterized plant material can be rapidly compared to new plants from the latest genetic cross, cultivation practice, or processing method.

Spectral fingerprinting is based on direct analysis (no separation) of a sample extract using ultraviolet (UV) and visible (vis) absorption, mass (MS), or nuclear magnetic resonance (NMR) spectrometry or analysis of the solid material using infrared (IR) or near-infrared (NIR) spectrometry (*1*−*7*). Chromatographic profiling employs a separation of the plant extract (or volatile components) by gas (GC) or liquid chromatography (LC) or gel or capillary electrophoresis (CE) with, most commonly, UV, fluorescence (F), or MS detection (*1*−*7*). In both cases, the comprehensiveness of the comparison is dependent on the extraction solvent and procedure that is used. In both cases, an integrated analysis of the chemical composition of the samples requires the use of pattern recognition programs.

Spectral fingerprints, regardless of the means of acquisition, are highly complex, representing the sum of the spectra of each compound present in a sample. In general, it is very difficult to identify, let alone quantify, individual compounds. While identification is sometimes attempted with MS fingerprints, the results are unreliable and chromatographic separation is required to obtain accurate results.

Principal components analysis (PCA) is the most commonly used pattern recognition program for unstructured analysis (*8*). Recently, Harrington et al. (*9*, *10*) reported on the use of analysis of variance (ANOVA)-PCA as a means of isolating experimental factors prior to PCA. This method constructs submatrices of the data for each factor that can be more easily interpreted, visually and statistically, by PCA. Harnly's group (*11*, *12*) reported a variation of ANOVA-PCA that uses the submatrices to compute the relative variance contributed by each factor.

Recent studies have compared the use of UV, vis, and MS spectra of aqueous methanol (60% MeOH and 40% $H_2O$)

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