# Evaluation of Smoky Taste in Cocoa Powder

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The aim of this study was to determine the levels of nine phenols (phenol, guaiacol derivatives, xylenols, and cresols) by using a GC/MS technique in smoked samples under control, commercial samples taken from contaminated batches, and uncontaminated samples. The smoky taste of cocoa powder may have two origins: drying and storage. The sample was steam distilled, extracted with ethyl ether, concentrated, and chromatographed on a 50-m OV-351 fused silica column. The physicochemical data obtained were related to sensory evaluation and submitted to multivariate distribution (Mahalanobis distance) and Pearson Chi-squared test. The discriminatory phenols identified were phenol, 3-methylphenol (*m*-cresol), 2,3-dimethylphenol (2,3-xylenol), 3-ethylphenol, 4-ethylphenol, and total phenols. The results obtained imply that uncontaminated smoked cocoa samples should have the following maximum concentrations: phenol, 2 mg/kg; 3-methylphenol, 0.9 mg/kg; 2,3-dimethylphenol, 0.55 mg/kg; 3-ethylphenol, 0.90 mg/kg; 4-ethylphenol, 0.70 mg/kg; and total phenols, 9.6 mg/kg.

**Keywords:** *Cocoa; smoky; phenolic compounds; sensory evaluation*

## INTRODUCTION

The technologic process applied to the freshly collected cocoa beans includes two fundamental operations: fermentation and drying. The fermentation is indispensable to reduce astringency, acidity, and bitternes of cocoa (Serra Bonvehí and Ventura Coll, 1997a,b), generating at the same time the aromatic precursors that will develop during the roasting process. After the fermentation, cocoa beans have an approximate water content of 50 g/100 g. It is necessary to preserve cocoa beans, reducing their water content to 6−7 g/100 g, by drying (Hor et al., 1984). The drying also enhances product preservation, by blocking enzymatic reactions and limiting the number of microorganisms (Ribeiro and Lopez, 1983; Schwan et al., 1995). Insufficiently dried cocoa is quickly degraded by microorganism action (fundamentally fungi) and enzymes (lipoxygenase, lipase, peroxidase, and polyphenol oxidase) (Villeneuve et al., 1985). Natural drying is difficult to obtain and the heat is irregularly distributed. For that reason artificial drying is applied (Borges et al., 1981). During drying, cocoa beans can be contaminated by smoke originating from badly conditioned dryers, and during storage too. The possible sources of smoky cocoa are numerous and include polluted air and water, mode of cooking, type of fuel (wood, diesel, etc), wood composition, and smoke generation conditions during processing. The smoke is a complex mixture of >1000 compounds, of which ∼400 have been identified (Tóth and Potthast, 1984; Maga, 1992). Among these compounds are phenols, carbonyl compounds, alcohols, organic acids, and others that contribute to the typical flavor, color, and taste. However, during the thermal decomposition of the shavings undesirable compounds are also formed, namely polycyclic aromatic hydrocarbons (PAHs), which are regularly found in smoked fishery products (Maga, 1986; Gomaa et al., 1993). The presence of benzo[*a*]pyrene and other carcinogenic PAHs in food has received considerable attention over the past three decades (Maga, 1988). Cocoa beans, rich in fatty matter (50−58 g/100 g), easily fix the smoke compounds, making it difficult to remove. Artificial drying reduces the processing time and yields a more homogeneous product but increases acidity and incorporates a fruity taste to cocoa (Jacquet et al., 1980). It is convenient to dry at a moderate temperature (<80 °C), because the more the temperature increases, the larger is the retention of acidity in the cotyledons (Jacquet et al., 1980). The drying conditions to comply with are as follows: a temperature of 65−70 °C (17−18 h), thickness 23−27 cm, and a moderate air flow of 0.4−0.5 m/s to avoid "caking". The results indicated that (a) there is a significant correlation between cocoa bean porosity and the respective drying time and (b) the relationship between porosity and moisture content varies with the drying air temperature (Prado et al., 1981). Although free phenols can be analyzed by gas chromatography and liquid chromatography, some researchers prefer to prepare methyl ether derivatives of phenol extracts and analyze the anisoles by electron capture gas chromatography (EC-GC) (Lee et al., 1984). Phenolic constituents are believed to contribute to both the flavor and aroma of tobacco smoke (Tomkins et al., 1984; Clark and Bunch, 1996) and smoked fishery products (Karl and Lienemann, 1996). Since synergistic and antagonistic processes occur, it is desirable to achieve a multivariate statistical procedure that allows the sensory attributes from the volatile compounds to be related. The procedure selected was multidimensional scaling (MDS) (Schiffman et al., 1981). The present work is part of a study regarding the nature of the primary characteristic aroma of roasted cocoa powder and about phenolic compounds incorporated during drying.

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**Table 1. Chromatographic Data (GC/FID and GC/MS)[a]**

| compd no. | compd name | RT | RRT | FR | ion monitoring |
|---|---|---|---|---|---|
| + | 4-ethylpyridine | 8.47 ± 0.27 | 1 | 1 | |
| **1** | 2-methoxyphenol | 15.45 ± 0.35 | 1.82 ± 0.03 | 1.20 | *124*, 94, 81 |
| **2** | phenol | 18.76 ± 0.31 | 2.21 ± 0.02 | 0.81 | *95*, 66 |
| **3** | 3-methylphenol | 19.10 ± 0.29 | 2.26 ± 0.03 | 0.96 | *108*, 107, 79, 77 |
| **4** | 4-methylphenol | 19.91 ± 0.30 | 2.35 ± 0.02 | 0.97 | *108*, 107, 79, 77 |
| **5** | 2,3-dimethylphenol | 21.07 ± 0.36 | 2.49 ± 0.03 | 0.93 | *122*, 107, 91 |
| **6** | 3-ethylphenol | 21.81 ± 0.31 | 2.57 ± 0.02 | 0.70 | 122, *107*, 94, 77 |
| **7** | 4-ethylphenol | 23.40 ± 0.31 | 2.76 ± 0.02 | 0.89 | 122, *107*, 94, 77 |
| **8** | 3,4-dimethylphenol | 24.70 ± 0.34 | 2.92 ± 0.03 | 0.98 | *122*, 107, 91, 77 |
| **9** | 3,5-dimethylphenol | 25.26 ± 0.29 | 2.98 ± 0.03 | 0.96 | *122*, 107, 91, 77 |

[a] RT, absolute retention time; RRT, relative retention time; FR, relative response coefficient; +, internal standard.

## MATERIALS AND METHODS

**Samples.** The fermentation and drying processes were performed according to the recommendations of the Comissao Executiva do Plano da Lavoura Cacaueira (CEPLAC) (1980). Three groups, totaling 30 samples of nonalkalinized cocoa powder (10−12% cocoa butter), were of different origins (Ghana, Ivory Coast, Nigeria, Brazil, Equador). The groups consisted of 10 samples correctly processed, 10 samples dried and poorly smoked, and 10 samples strongly contaminated with direct smoke. An external smoke generator (type MC3, Maurer, Germany) was utilized. The smoke is generated from shavings of wood in an electrical oven and carried by air flow to a chamber containing the samples. The smoking conditions to comply with are as follows: air temperature of 65−70 °C; relative humidity (RH) between 40 and 60%; air flow of 0.4−0.5 m/s; total smoking times of 10 min (poorly smoked samples) and 30 min (strongly smokes samples). Samples were preserved at 0−5 °C and analyzed as soon they arrived at the laboratory. Analyses were carried out in triplicate.

**Physicochemical Analyses.** *Reagents and Standards.* Solvents were of analytical (Panreac, Barcelona, Spain) and GC (Merck, Darmstadt, Germany) grades. Laboratory deionized water was further purified using a vacuum filter (0.45 $\mu$m, Schleicher & Schuell, Dassel, Germany). Standard phenols 4-ethylpyridine, 2,3-dimethylphenol, 3,4-dimethylphenol, 3,5-dimethylphenol, 3-ethylphenol, 4-ethylphenol, and phenol were obtained from Fluka Chemika (Buchs, Switzerland), 99+% purity; standard phenols 3-methoxyphenol, 3-methylphenol, and 4-methylphenol were purchased from Sigma Chemical Co. (St. Louis, MO), 99+% purity.

*Phenolic Compounds.* The method used to determine phenolic compounds was adapted from the method proposed by Guyot et al. (1986). Cocoa powder (20 g) was homogenized with 40 mL of water in an ultrasonic bath. The mixture was steam distilled, and the distillate was collected in a trap of 50 mL of ethyl ether. The condenser was maintained at 0 °C, and distillation was continued until 100 mL of distillate was collected. NaCl (10 g) was added to the distillate, and the resulting solution was transferred to a separatory funnel. Ethyl ether (50 mL) was added, mixed by agitating, and allowed to separate. The ethylic phases were joined and washed three times with 50 mL of 0.1 M $KH_2PO_4$ (pH 5.80). Anhydrous $MgSO_4$ (10 g) was added, and the solution was allowed to stand for 30 min before it was filtered and concentrated to dryness under reduced pressure (300 mmHg) at 40 °C. Internal standard (0.2 mL) (0.1 g of 4-ethylpyridine in 100 mL of $Cl_3CH$) along with $Cl_3CH$ (0.5 mL) was added to the final extract (Silwar et al., 1986; Hashim and Chaveron, 1994).

*High-Resolution Gas Chromatography (HRGC).* A Hewlett-Packard model 5890 gas chromatograph equipped with an HP model 7673 automatic sampler, a flame ionization detector (FID), and an integrator (HP model 3393A) was used. Separation was accomplished with an OV-351 column (50 m × 0.32 mm i.d. × 0.20-$\mu$m film thickness) (Supelco, Inc., Bellefonte, PA). GC conditions were as follows: 1 $\mu$L splitless injection (75-s valve delay); oven programmed from 70 to 210 °C, at a rate of 5 °C/min; 240 °C injector temperature; 250 °C detector temperature; helium as carrier gas at a flow of 1.5 mL/min.

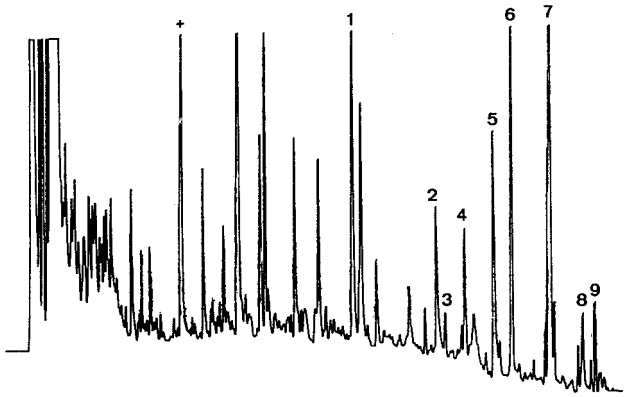


**Figure 1.** GC/FID phenol profiles of cocoa powder.

The relative amount of each compound were expressed by the ratio of its total peak area with that of the internal standard. All single phenolic compound standards were dissolved in cloroform, each at a concentration of 100 mg/L, and diluted with cloroform to 1, 4, 10, and 20 mg/L concentrations. All solutions were stored at 5 °C in the dark prior to use.

*Gas Chromatography/Mass Spectrometry (GC/MS).* When necessary, confirmation of phenolic compounds was achieved by GC/MS. The column (see above) was directly connected to a Hewlett-Packard 5988 column quadruple mass spectrometer. Mass spectra in the electron-impact mode (MS-EI) were generated at 7O eV with a source temperature of 270 °C and a scan range of 30−600 amu at a rate of 1.3 scans/s. Purified helium was the carrier gas. Spectral recording throughout electron impact was automatically performed with the HP 5970C MS Chemstation analytical workstation. Mass spectrometric detection was made in the selected ion mode. Selected mass spectral ions monitored are listed in Table 1. Peak identifications were based on comparison of mass spectra of unknowns with those of authentic standard compounds under identical experimental conditions.

*Sensory Evaluation.* Sensory evaluation was carried out by a taste panel under the conditions of the International Standard (ISO, 1985). Ten staff members, 5 women and 5 men, were selected as the sensory panel. All panelists had been screened for sensitivity to smoked flavor. The panel training program was designed in two phases. Phase 1 provided an orientation to base principles of sensory analysis. Phase 2 focused on the sensory characteristics of typical smoked cocoa bean. Panelists came together for 30-min round-table discussion sessions during which assessment techniques and terminology were developed. Panel evaluation was carried out by paired comparison tests. Panelists were asked to determine which sample of the pair had highest intensity and to evaluate the acceptability (1) or unacceptability (0) of a sample. The sensorial attributes were smell and taste.

*Statistical Analyses.* The results and the sensory evaluation were submitted to analyses of variance and the multivariate distribution made by Mahalanobis distance (Hernández and Rutledge, 1994; Naes and Risvik, 1996), evaluated as Chi-squared, using the Systat computer package (Wilkinson, 1989).

**Table 2. Phenol Compounds in Uncontaminated Cocoa Powder**

| | sample no. | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| compd | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | $X$ | SD | $V_{max}$ | $V_{min}$ |
| 2-methoxyphenol | 2.71 | 2.11 | 3.01 | 1.75 | 3.17 | 1.81 | 1.87 | 3.22 | 1.75 | 2.27 | 2.37 | 0.61 | 3.22 | 1.75 |
| phenol | 1.12 | 1.12 | 0.92 | 0.84 | 1.09 | 0.87 | 1.70 | 1.85 | 0.87 | 1.19 | 1.14 | 0.36 | 1.85 | 0.84 |
| 3-methylphenol | 0.77 | 0.61 | 0.45 | 0.39 | 0.47 | 0.33 | 0.71 | 0.67 | 0.57 | 0.71 | 0.57 | 0.15 | 0.77 | 0.33 |
| 4-methylphenol | 1.21 | 1.37 | 1.27 | 1.17 | 1.19 | 0.89 | 1.09 | 0.95 | 0.78 | 1.07 | 1.10 | 0.18 | 1.37 | 0.78 |
| 2,3-dimethylphenol | 0.35 | 0.31 | 0.35 | 0.47 | 0.27 | 0.39 | 0.28 | 0.25 | 0.19 | 0.29 | 0.32 | 0.08 | 0.47 | 0.19 |
| 3-ethylphenol | 0.38 | 0.35 | 0.71 | 0.28 | 0.41 | 0.55 | 0.61 | 0.39 | 0.41 | 0.57 | 0.47 | 0.14 | 0.71 | 0.28 |
| 4-ethylphenol | 0.47 | 0.42 | 0.57 | 0.37 | 0.42 | 0.41 | 0.61 | 0.41 | 0.39 | 0.47 | 0.45 | 0.08 | 0.61 | 0.37 |
| 3,4-dimethylphenol | 0.28 | 0.25 | 0.35 | 0.12 | 0.19 | 0.32 | 0.37 | 0.29 | 0.22 | 0.31 | 0.27 | 0.08 | 0.37 | 0.12 |
| 3,5-dimethylphenol | 0.21 | 0.19 | 0.28 | 0.15 | 0.27 | 0.29 | 0.41 | 0.31 | 0.27 | 0.35 | 0.27 | 0.08 | 0.41 | 0.15 |
| total phenols | 7.50 | 6.53 | 7.96 | 5.54 | 7.48 | 5.86 | 7.65 | 8.34 | 5.45 | 7.23 | 6.95 | 1.04 | 8.34 | 5.45 |

**Table 3. Phenol Compounds in Poorly Smoked Cocoa Powder**

| | sample no. | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| compd | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | $X$ | SD | $V_{max}$ | $V_{min}$ |
| 2-methoxyphenol | 3.47 | 3.75 | 4.31 | 3.31 | 4.15 | 3.19 | 4.25 | 3.87 | 4.07 | 3.98 | 3.83 | 0.40 | 4.31 | 3.19 |
| phenol | 2.10 | 2.37 | 3.71 | 2.71 | 3.47 | 2.95 | 3.37 | 3.47 | 3.20 | 2.90 | 3.03 | 0.52 | 3.71 | 2.10 |
| 3-methylphenol | 0.97 | 1.10 | 1.31 | 0.87 | 1.17 | 1.08 | 1.21 | 1.19 | 1.21 | 1.09 | 1.12 | 0.13 | 1.31 | 0.87 |
| 4-methylphenol | 1.37 | 1.45 | 1.71 | 1.57 | 1.29 | 1.17 | 1.63 | 1.56 | 1.59 | 1.45 | 1.48 | 0.17 | 1.71 | 1.17 |
| 2,3-dimethylphenol | 0.41 | 0.47 | 0.51 | 0.45 | 0.57 | 0.53 | 0.61 | 0.49 | 0.57 | 0.43 | 0.50 | 0.07 | 0.61 | 0.41 |
| 3-ethylphenol | 0.71 | 0.92 | 0.89 | 0.79 | 0.97 | 0.85 | 0.95 | 0.85 | 0.93 | 0.77 | 0.86 | 0.09 | 0.97 | 0.71 |
| 4-ethylphenol | 0.57 | 0.61 | 0.71 | 0.68 | 0.59 | 0.65 | 0.59 | 0.63 | 0.71 | 0.65 | 0.64 | 0.05 | 0.71 | 0.57 |
| 3,4-dimethylphenol | 0.47 | 0.57 | 0.63 | 0.51 | 0.71 | 0.67 | 0.75 | 0.59 | 0.63 | 0.53 | 0.61 | 0.09 | 0.75 | 0.47 |
| 3,5-dimethylphenol | 0.55 | 0.68 | 0.71 | 0.61 | 0.65 | 0.75 | 0.61 | 0.71 | 0.77 | 0.61 | 0.67 | 0.07 | 0.77 | 0.55 |
| total phenols | 10.6 | 11.9 | 14.5 | 11.5 | 13.5 | 11.8 | 14.0 | 13.4 | 13.0 | 12.4 | 12.7 | 1.23 | 14.5 | 10.6 |

**Table 4. Phenol Compounds in Strongly Smoked Cocoa Powder**

| | sample no. | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| compd | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | $X$ | SD | $V_{max}$ | $V_{min}$ |
| 2-methoxyphenol | 5.12 | 6.30 | 5.87 | 6.53 | 4.67 | 7.71 | 4.81 | 3.87 | 5.57 | 6.07 | 5.65 | 1.09 | 7.71 | 3.87 |
| phenol | 3.67 | 4.25 | 4.10 | 4.81 | 5.07 | 6.37 | 4.67 | 4.37 | 4.96 | 4.15 | 4.64 | 0.75 | 6.37 | 3.67 |
| 3-methylphenol | 1.53 | 1.95 | 1.75 | 2.07 | 2.25 | 1.75 | 1.25 | 1.97 | 2.07 | 2.37 | 1.90 | 0.34 | 2.37 | 1.25 |
| 4-methylphenol | 2.33 | 2.57 | 2.10 | 2.72 | 3.07 | 1.96 | 2.31 | 2.01 | 2.15 | 2.86 | 2.41 | 0.38 | 3.07 | 1.96 |
| 2,3-dimethylphenol | 1.77 | 2.12 | 1.55 | 1.97 | 2.15 | 3.17 | 3.87 | 1.97 | 2.71 | 3.21 | 2.45 | 0.75 | 3.87 | 1.55 |
| 3-ethylphenol | 2.17 | 2.01 | 1.78 | 2.27 | 2.61 | 3.35 | 4.07 | 1.93 | 3.07 | 2.81 | 2.54 | 0.81 | 4.07 | 1.78 |
| 4-ethylphenol | 1.97 | 2.37 | 1.87 | 2.18 | 2.57 | 2.96 | 3.17 | 2.15 | 2.15 | 2.76 | 2.41 | 0.43 | 3.17 | 1.87 |
| 3,4-dimethylphenol | 0.66 | 0.81 | 0.71 | 0.97 | 0.77 | 0.81 | 0.71 | 0.69 | 0.57 | 0.71 | 0.74 | 0.11 | 0.97 | 0.57 |
| 3,5-dimethylphenol | 0.78 | 0.95 | 0.88 | 1.07 | 0.83 | 0.95 | 0.57 | 0.71 | 0.87 | 1.07 | 0.87 | 0.16 | 1.07 | 0.57 |
| total phenols | 20.0 | 23.3 | 20.6 | 24.6 | 24.0 | 29.0 | 25.4 | 19.7 | 24.1 | 26.0 | 23.7 | 2.92 | 29.0 | 19.7 |

## RESULTS AND DISCUSSION

Table 1 shows the detected chromatographic peaks in elution order, average absolute retention time (RT), average retention time (RRT), relative response coefficients [relative RC = (compound concentration (ppm)/internal standard peak area)/(compound concentration (ppm)/internal standard concentration (ppm))] for the various volatile constituents, and name attributed to each identified compound. The following compounds were identified: (1) phenol; (2) phenolic ethers (xylenols and cresols). The identification and quantification of the phenolic fraction required distillation−extraction, purification, and gas chromatography (GC/FID and GC/MS). Five replicate injections were made to obtain the precision of the technique. The precision was acceptable, with an average percent relative standard deviation of <10%. The recovery was established by adding increasing amounts of phenolic compounds covering the concentration range present in the samples analyzed (5−10 mg/kg) to an uncontaminated cocoa powder sample. The mean recoveries of phenol derivatives were ≈80%. A typical chromatogram (Figure 1) shows the resolution of phenolic compounds. Phenolic compounds appear in the chromatogram starting after 15 min. Nine compounds were identified using the described methods. Tables 2−4 show data from phenolic compounds, 2-methoxyphenol, phenol, and 4-methylphenol being the most abundant. The results obtained coincide with those of Guyot et al. (1986). The composition of the phenolic compounds in cocoa beans is influenced by external factors: the drying processes and storage. When the temperature and the drying process period are excessively high or long, the phenolic compound content increases (Tables 2−4). The values obtained in Table 2 are typical of correctly processed cocoa beans. The values in Tables 3 and 4 correspond to incorrectly processed cocoa beans (Table 3, poorly smoked, and Table 4, strongly smoked). The analyzed samples had a homogeneous composition of phenolic compounds. The aim of the statistical analysis was to distribute the cocoa samples bearing in mind the smoky taste attributed to phenolic compounds (10 variables: individual identified phenolic compounds plus the total) and sensory acceptance. The Pearson Chi-squared test performed using results from Tables 2−4 showed the existence of significant differences ($P < 0.05$) between acceptable (Table 2) and unacceptable samples (Tables 3 and 4) in terms of analytical and sensory evaluation. Although the analysis reported that samples of cocoa powder correctly processed have been shown to be markedly different from cocoa powder inadequately smoked, sensorially accepted samples (Table 2) and poorly smoked

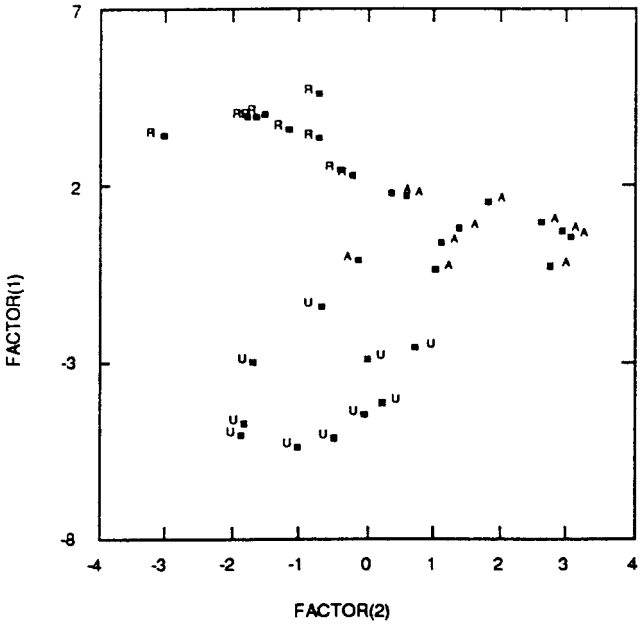


**Figure 2.** First two factors of multidimensional scaling of attribute perceptions: (A) not smoked; (R) poorly smoked; (U) strongly smoked.

samples (Table 3) were statistically analyzed to determine the limiting content of phenolic compounds that indicated when a sample was smoked. Due to the nature and the amount of data generated, multivariate statistics (chemometrics) was used to extract the information presented (Table 2−4) and draw valid conclusions. The principal strategy of these methods was to consider each experimental variable as a coordinate axis in a *k*-dimensional space ($k$ = number of variables), the measurement space. Each sample was described by a vector representing the values of the experimental variables and represented as a point in this space. Using the same measured variables, a set of objects form a swarm of point in *M*-space and samples similar to each other would be near each other, so that distance would constitute a measure of similarity/dissimilarity. The principal components can be plotted, thus revealing natural groupings that can be utilized in classification. Principal component analysis (PCA) is now a well-established tool for the interpretation of chemical data. The major step in a PCA is the extraction of the eigenvectors from the variance−covariance matrix to obtain uncorrelated new variables called principal components (PCs), which span the maximum variance in the data set. The PCs are linear combinations of all of the original variables. The PC loadings are coefficients of the correlation between the variable vectors and the PCs. The PC scores are the coordinates of the sample points on the PCs. The original matrix, composed of 30 lines (the cocoa powder samples) and 10 columns (variable phenol compounds), was centered and standardized. Figure 2 shows a classical representation of the scores on PC1 (factor 1) and PC2 (factor 2) (55% of total variance). Peaks 3 (3-methylphenol), 6 (3-ethylphenol), and 7 (4-ethylphenol) make a large contribution to the first PC. The second PC is not dominated by any one particular component, but phenol and 2,3-dimethylphenol have the highest coefficient in this linear combination. A univariate *F* test was performed to differentiate discriminant variables. The discriminant phenolic compounds were phenol, 3-methylphenol (*m*-cresol), 2,3-dimethylphenol (2,3-xylenol), 3-ethylphenol, 4-ethylphenol, and total phenols. A canonical correlation was performed using the discriminant compounds to analyze the relationhip between the two sets of variables to see how the two sets relate to each other. Model verification was performed including the unaccepted samples (Table 5). Samples were well classified; of the 10 poorly smoked samples, only 1 sample was grouped as acceptable and the other 9 were grouped as unacceptable. The Pearson Chi-squared test was performed to determine whether obseved values were not significantly different ($P < 0.05$) from predicted values in terms of analytical and sensory evaluation. The results of applying MDS to the data sets of phenol compounds and sensory attributes are displayed in Figure 2. Finally, Mahalanobis distances were calculated, and the limiting value was defined (maximum distance between accepted and poorly smoked). We can infer that optimally processed cocoa samples should have a maximum total of phenolic compounds of 9.6 mk/kg. On the basis of these results, phenol compound content has been related to the sensory score, and the maximum values of these parameters (phenol, 2 mg/kg; 3-methylphenol, 0.90 mg/kg; 2,3-dimethylphenol, 0.55 mg/kg; 3-ethylphenol, 0.90 mg/kg; 4-ethylphenol, 0.70 mg/kg; and total phenols, 9.6 mg/kg) could be used as an objective specification of the acceptance of cocoa powder.

**Table 5. Observed and Predicted Distribution of Samples**[a]

| | sample | | | |
|---|---|---|---|---|
| distribution | A | R | U | total |
| A | 10 | 0 | 0 | 10 |
| R | 1 | 9 | 0 | 10 |
| U | 0 | 0 | 10 | 10 |
| total | 11 | 9 | 10 | 30 |

[a] A, adequate; R, poorly smoked; U, highly smoked.

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