



Volatile organic compound profile of roasted and unroasted fine aroma cocoa genotypes from Peru

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Abstract

Cocoa (*Theobroma cacao* L.) is one of Peru's main export products. In the last years, the production of fine aroma cocoa has increased, and the market has preference for them instead of cultivar clones like CCN51. Fine aroma cocoa is a heterogeneous population, but some genotypes have started to be selected. This study aimed to evaluate the chemical properties and volatile organic compound (VOC) profile of different fine aroma cocoa genotypes and CCN51. The chemical composition—including moisture, fat, protein, ash, carbohydrate, pH, fermentation index and total phenolic compounds—was determined using standard analytical procedures. VOC were analyzed using SPME/GC-MS. Protein content varied among genotypes, with ABL01 showing the highest percentage. Fat content also ranged widely, with ABL01 and JBB04 representing the highest and the lowest values, respectively. Significant differences in ash and carbohydrate contents were also observed. The pH values suggested that fermentation was generally adequate, although some genotypes showed potential deficiencies. Fine aroma cocoa (FAC) genotypes exhibited lower phenolic compound content compared to the commercial clone CCN51. VOC analysis revealed compositional differences, with certain compounds contributing more prominently to the variation of specific genetic groups profile. These findings suggest that there exists a huge variability in VOC and other chemical properties of fine aroma cocoa genotypes and it is expected that data generated about roasted and no roasted beans will be useful for future research.

Keywords Biodiversity · CCN51 · GC-MS · Phenolic compounds · Volatile organic compounds

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Introduction

Cocoa, the primary raw material for chocolate production, owes much of its sensory value to its volatile compound profile [1]. Global cocoa production is predominantly composed of standard cocoa, mainly represented by the Forastero variety, which accounts for approximately 95–97% of total output. In contrast, fine aroma cocoa (FAC), which includes the Trinitario and Criollo varieties—characterized by medium and high aromatic quality, respectively—makes up only 5–6% of global production [2]. Criollo cacao trees have a lower yield and are more susceptible to pests and diseases. Trinitario cacao trees are a hybrid species that combines traits of Criollo and Forastero types, resulting in a less pronounced fragrance, but higher yields and resistance to pests and diseases [5]. Fine aroma cocoa is ideal to produce high-quality or premium chocolates, making them up to five times more expensive than Forastero cocoa [3, 4]. In the last years, the production and commercialization of FAC has increased in the northern region of Peru. As it is formed by a heterogeneous population, agricultural cooperatives such as APROCAM, that has at least 13 members with 0.56–3.3 ha of FAC, have started to select some elite genotypes according to production and sanitary conditions. Those accessions were propagated for future evaluation. VOC profile of these accessions is lacking, and these compounds are influenced by the fermentation process. During cocoa beans fermentation, many volatile compounds (such as esters, alcohols and short-chain fatty acids), along with chocolate flavour precursors (including reducing sugars and amino acids), are formed [6]. Free amino acids and short-chain peptides, precursors of VOC, are formed through the proteolysis of seed proteins [7]. Additionally, reducing sugars released during fermentation play an important role in the Maillard reaction that occurs during roasting, primarily leading to the formation of aldehydes and pyrazines [8]. Together with esters, alcohols and ketones contribute to the cocoa, nutty, malty, fruity, and floral notes of cocoa products [9]. If fermentation

does not occur or is incomplete, the typical chocolate flavours are not developed during roasting. Consequently, the final product may taste excessively bitter and astringent due to its high polyphenol content and the limited formation of aroma precursors [10]. The different volatile and non-volatile compounds produced during the fermentation and drying process are considered as the indicative of the cocoa beans' quality [11]. Flavour is essential for the acceptability of chocolates, which is influenced by the release of volatiles for its perception [12]. The aromas produced by fine aroma cocoa beans include notes of fresh and ripe fruits, flowers, herbs and woods, as well as sweet and nutty nuances, together with monoterpenes such as linalool, and rich and balanced chocolate-based notes following fermentation and roasting of beans [13].

In this sense, the objective of this work was to determine the VOC profile and chemical composition of roasted and unroasted beans of fine aroma cocoa genotypes (*Theobroma cacao* L.) grown in the Amazon region.

Materials and methods

Study material

The material consisted of samples of fermented and dried native fine aroma cocoa beans (*Theobroma cacao* L.) of approximately 1 kg, obtained from six elite genotypes (ABL01, ABL03, VVA01, MRC05, MRC10 and JBB04) selected from fields of farmers of the APROCAM Cooperative and their technicians according to apparent agronomic characteristics such as seed quality, production, plant structure. Information received from the Cooperative is presented in Table 1. These plant trees are 14–28 years old, with plant-to-plant distance of 3 × 3 m, are in regions where temperatures of 22 °C and 32 °C are prevalent. Clone CCN51 was used as a control sample, because it is most widely cultivated and commercially distributed. Its origin

Table 1 Selected plant trees information

Genotype	Localization	Altitude in m.a.s.l.	Plant age	Plant height (m)	Pod color	Pod number per plant	Diseased pod percentage	Pod index (number of pods to obtain 1 kg of dry cocoa beans)
CCN51	Bagua and Aramango	n.d.	n.d.	n.d.	Red	n.d.	n.d.	n.d.
ABL01	Bagua, Copallin District, C.P. Pan de azúcar	1086	14	3.7	Green	114	8	39
ABL03	Bagua, Copallin District, C.P. Pan de azúcar	1086	14	3.3	Red	173	1.84	35
JBB04	Bagua, La Peca District	1058	n.d.	5.3	Green	190	1.75	43
MRC05	Bagua, Copallin District, C.P. Lluhuana	918	28	6.5	Green	98	8.14	49
MRC10	Bagua, Copallin District, C.P. Lluhuana	898	28	5.6	Red	55	35	53
VVA01	Bagua and Copallin	1087	n.d.	3	Green	75	4	39

n.d. = no determined

is aleatory from several producers. Harvest happens mainly from March to June and from September to November.

Post harvest process

In the cooperative cocoa beans collected were fermented in stainless steel covered wood boxes with capacity to contain up to 50 kg of beans. During the process the cocoa beans are mixed and transferred to a contiguous box every 48 h. The process usually takes 7 days, but the cooperative employees experimentally evaluate if the beans are ready to be dried. The fermented beans were dried in a cocoa drying tunnel with frequent turning and mixing until 7% of moisture. When fine flavour cocoa is fermented, it is separated from the CCN51 clone. Then, they were sent to the laboratory and frozen until analysis. To obtain the nibs (roasted beans), a Venticell ECO line oven (BMT Medical Technology) was used to expose the seeds to 110 °C for 20 min.

Chemical analysis

Moisture, fat, protein and ash contents were determined in unroasted cocoa beans following AOAC methods [14].

Moisture was measured using AOAC 931.04. Two grams of ground cocoa were placed in a drying oven at 105 °C for 16 h. After drying, the samples were cooled in a desiccator and weighed until constant weight was reached.

Fat content was determined using AOAC 963.15. Around 5 g of ground cocoa were wrapped in filter paper and placed in a Soxhlet extractor. As solvent 150 of petroleum ether was used. Following extraction, the solvent was evaporated, and the flask containing the fat residue was dried at 100 °C to remove traces of solvent. The percentage of fat was calculated gravimetrically. Protein content was determined by the Kjeldahl method (AOAC 970.22) with modifications. One gram of sample was digested with 10 mL of concentrated sulfuric acid and 5 g of catalyst in a digestion unit. The digest was diluted, neutralized with 32% NaOH, and distilled. The distillate was collected in 50 mL of boric acid solution and titrated with 0.25 N HCl. Crude protein was calculated by multiplying total nitrogen by a factor of 6.25. Ash content was determined using AOAC 972.15. Two grams of dry cocoa were incinerated in a muffle furnace at 600 °C for 4 h. After cooling in a desiccator, the remaining inorganic residue was weighted, and the result expressed as a percentage of ash. Total carbohydrate content was estimated by difference [15], subtracting the sum of moisture, fat, protein, and ash percentages from 100%.

The pH of the fermented and dried samples was determined using AOAC 970.21 [14]. Ten grams of ground cocoa were mixed with 90 mL of boiling distilled water in

a beaker. After filtration and cooling to 20–25 °C the pH of the filtrate was measured using a calibrated pH meter.

The fermentation index (FI) was determined according to the method of Gourieva and Tserevitinov [16]. A mixture of 0.5 g ground cocoa in 50 mL of methanol: HCl (97:3, v/v) was made and stored at 8 °C for 16–18 h. The extract was filtered, and absorbance was measured at 460 and 530 nm using a spectrophotometer (Unico UV2100PU). The FI was calculated as the ratio of absorbance at 460–530 nm:

$$FI = A_{460}/A_{530} \quad (1)$$

Total phenolic content was determined using the Folin-Ciocalteu method [17]. Extraction of 100 mg defatted cocoa samples was made with 5 mL of 70% acetone, shaken for 20 min, and centrifuged at 5000 rpm. The supernatant (250 µL) was mixed with 1.25 mL of Folin-Ciocalteu reagent and 1 mL of 7.5% sodium carbonate and 1.2% sodium tartrate solution. After incubating in the dark for 2 h at room temperature, absorbance was measured at 765 nm. A tannic acid standard curve was used, and results were expressed as mg of tannic acid equivalents per gram of cocoa (mg TAE/g).

Volatile organic compounds (VOC) by SPME-GC-MS

VOC were analyzed in cocoa beans before and after roasting using solid-phase microextraction (SPME) and gas chromatography-mass spectrometer (GC-MS), as described by Moreira et al. [18], with some modifications.

Cocoa samples were manually dehulled and ground in a porcelain mortar using liquid nitrogen. Four grams of ground sample were placed in a 20 mL vial sealed with an aluminum cap and PTFE/silicone septum. A 50/30 µm Divinylbenzene/Carboxen/Polydimethylsiloxane (DVB/CAR/PDMS) SPME fiber was used. Sample headspace equilibrium was reached after 15 min at 60 °C, followed by fiber exposure to the headspace at the same temperature for 30 min. Chromatographic analysis was performed using an Agilent 7890B gas chromatograph coupled with a 5977B mass selective detector (MSD) and a DB-5MS UI capillary column (60 m × 0.25 mm × 1.0 µm, Agilent®). The oven was initially held at 50 °C for 5 min, then ramped at 4 °C/min to 250 °C. Helium was used as carrier gas at a constant flow rate of 1.1 mL/min. The injector (split 1:1), transfer line, ion source and quadrupole were maintained at 250 °C, 250 °C, 230 °C and 150 °C, respectively. Data were acquired in scan mode using electron impact ionization at 70 eV, scanning a mass range of 35–400 amu.

Chromatographic peaks were deconvoluted using Agilent MassHunter Unknowns Analysis software. VOC were identified by comparison with the NIST 2017 mass spectral library and by calculating the linear retention index (LRI)

using retention times from a standard mix of *n*-alkanes (C_{10} – C_{40}), injected under the same conditions as the samples. All VOC showing mass spectra with match factor $\geq 80\%$ were considered. Additionally, peak symmetry was checked individually for confirmation.

Volatile compounds were not quantified using specific external standards. Instead, a semi-quantitative approach was employed, in which the peak areas obtained from the chromatograms were used as indicators of relative abundance. This allowed the comparison of VOC levels among different treatments and genotypes. All samples were analyzed in triplicate, and only compounds detected in at least two out of three were considered as means of three replicates for statistical evaluation and discussion.

Statistical analysis

Differences among genotypes in moisture, protein, fat, ash, carbohydrate content, and total phenolic compounds were assessed using a parametric analysis of variance (ANOVA), followed by Tukey's test at a significance level of $p < 0.05$. Kruskal-Wallis test was applied for pH and fermentation index because it did not meet the assumption of normality. To identify specific pairwise differences, Dunn's post hoc test was performed using the Bonferroni correction method. Additionally, a pairwise Wilcoxon rank-sum test with Bonferroni adjustment was conducted to confirm the differences between genotype pairs. To identify sample groupings and explore relationships with volatile organic compounds (VOC), a Principal Component Analysis (PCA) was performed, followed by hierarchical cluster analysis, visualized using a heatmap. Cluster analysis was conducted using the Euclidean distance metric combined with the complete linkage clustering method to maximize group homogeneity. The selection of the most influential VOC in differentiating cocoa genotypes was performed in two stages: (i) calculation of the mean chromatographic peak area of each VOC within genotype groups, and (ii) selection of the 10 most influential VOC per group, based on the highest mean area.

These most relevant VOC were then used to construct the heatmap. The data were normalized (scale between 0 and 1) before clustering to minimize the effect of absolute magnitude differences between compounds. The heatmap was generated using `pheatmap()` function in R, with a blue-to-red color scale representing the minimum and maximum values, respectively. All variables were measured in triplicate, and the data were analyzed using RStudio [19]. Differences were considered statistically significant when $p < 0.05$, and different letters in the columns of Table 2 indicate statistically significant differences among genotypes.

Results

The results of the chemical analysis of the cocoa beans can be observed in Table 2. The moisture values were between 5.03% and 6.52%. It was found that the CCN51 ($14.51\% \pm 0.25\%$) had intermediate values in relation to ABL01 genotype ($16.19\% \pm 0.38\%$) that had the highest percentage of protein and the VVA01 genotype ($11.81\% \pm 0.66\%$) had the lowest percentage, with significant differences among them. Regarding the fat content, it was found that the ABL01 and VVA01 genotypes had the highest content with 29.54% and 27.79%; the JBB04 (21.37%) had the lowest content and showed significant differences with them. However, CCN51 clone did not show differences with them both, the genotypes with the highest and lower fat percentage. The ash percentages of the genotypes varied from 2.14 to 3.11%, for CCN51 and VVA01, respectively, with significant differences. For carbohydrates, the lowest value was for the ABL01 genotype ($45.61\% \pm 1.93\%$) and the highest for JBB04 ($56.67\% \pm 0.45\%$), and the CCN51 clone again was among them with $50.55\% \pm 3.08\%$ with significant difference with JBB04 but no with ABL01. Regarding pH, the highest value was found in the CCN51 with significant differences with the other genotypes, except ABL01 genotype, both with 5.4.

Table 2 Chemical properties of raw-unroasted cocoa beans of different genotypes

Parameters Genotypes	Moisture (%)	Protein (%)	Fat (%)	Ashes (%)	Carbohydrates (%)	pH	Fermentation index (FI)	Total pheno- lic com- pounds (mg TAE/g)
CCN51 (control)	5.68 ± 0.04^c	14.51 ± 0.25^{bc}	27.12 ± 3.16^{ab}	2.14 ± 0.01^d	50.55 ± 3.08^{bc}	5.4 ± 0.00^a	1.46 ± 0.03^c	125.40 ± 7.13^a
ABL01	6.11 ± 0.17^b	16.19 ± 0.38^a	29.54 ± 2.19^a	2.56 ± 0.07^{bc}	45.61 ± 1.93^c	5.4 ± 0.06^{ab}	2.10 ± 0.04^{ab}	69.89 ± 6.46^d
ABL03	5.85 ± 0.16^{bc}	13.64 ± 0.55^{cd}	26.54 ± 1.98^{ab}	2.66 ± 0.05^{bc}	51.31 ± 1.40^{ab}	5.1 ± 0.00^d	1.71 ± 0.01^{bc}	86.59 ± 5.15^c
JBB04	5.73 ± 0.15^c	13.49 ± 0.33^{cd}	21.37 ± 0.76^b	2.74 ± 0.13^b	56.67 ± 0.45^a	4.8 ± 0.06^e	1.38 ± 0.26^{de}	101.66 ± 6.33^b
MRC05	5.73 ± 0.07^c	12.83 ± 0.33^{de}	24.49 ± 2.18^{ab}	2.38 ± 0.14^{cd}	54.57 ± 2.14^{ab}	5.3 ± 0.00^c	2.57 ± 0.06^a	66.88 ± 3.57^d
MRC10	5.03 ± 0.05^d	15.09 ± 0.22^{ab}	24.57 ± 1.97^{ab}	2.58 ± 0.10^{bc}	52.73 ± 1.78^{ab}	5.1 ± 0.06^d	1.63 ± 0.03^c	105.65 ± 2.94^b
VVA01	6.52 ± 0.06^a	11.81 ± 0.66^e	27.79 ± 1.92^a	3.13 ± 0.17^a	50.75 ± 1.94^{bc}	5.3 ± 0.06^{bc}	1.54 ± 0.03^d	73.92 ± 2.57^{cd}

Results presented as mean values $\pm$ standard deviation. Different letters indicate statistically significant differences ($p < 0.05$) among genotypes

Cocoa beans with a fermentation index (FI) below 1.0 are considered under-fermented, whereas values above this threshold are generally interpreted as indicative of fully fermented beans [16]. However, FI values higher than 1.6 are considered over-fermented [20]. Genotypes CCN51, JBB04 and VVA01 had a good fermentation index with values of 1.46 ± 0.03 , 1.38 ± 0.26 and 1.54 ± 0.03 , respectively. However, genotypes ABL01 and MRC05 had FI of 2.10 ± 0.04 and 2.57 ± 0.06 , respectively, and were considered over-fermented beans; there seems to be an association with the pH found and, mainly, with the total phenolic compounds. Regarding the last parameter, the fine aroma cocoa (FAC) genotypes presented values between 66.88 ± 3.57 and 105.65 ± 2.94 mg TAE/g of cocoa, being lower statistically in relation to the commercial clone CCN51 (125.40 ± 7.13 mg TAE/g of cocoa). Genotype VVA01 behaved differently because it presented the lowest percentage of protein, the highest percentage of ash, one of the lowest total phenolic compounds and an adequate fermentation index. The Cooperative has standardized the fermentation process to seven days to ensure proper and consistent fermentation quality.

Figure 1 shows the principal component analysis (PCA), where four distinct clusters of the cocoa genotypes are observed. A first cluster includes the genotypes CCN51, MRC05, MRC10 and VVA01; the second cluster

is composed solely of ABL03; the third cluster includes ABL01; and the fourth cluster contains JBB04. The ABL03 genotype is of particular interest to cooperative officials due to its aromatic profile perceived during mucilage tasting.

The first two principal components (PC1 and PC2) explain 77.1% of the total variability observed in the 79 volatile organic compounds (VOC) identified in both unroasted and roasted beans. Including the third component (PC3), which accounts for an additional 9.3%, raises the total explained variance to over 86%. Most VOC are concentrated near the center of the PCA biplot, suggesting that they contribute broadly across genotypes. In contrast, VOC located farther from the center have stronger discriminatory power and contribute more distinctly to specific genotype clusters.

To further explore the relationship between VOC and genotypes, the ten most influential VOC for each genotype were selected based on their mean chromatographic peak area and contribution scores from the PCA. These are visualized in Fig. 2 as a heatmap, where rows represent VOC and columns represent genotypes.

Group 1 was primarily influenced by benzaldehyde (32, 111), heptan-2-yl acetate (8, 87), 2-pyridinealdoxime (17, 96), 2-heptanone (88), 2-nonanone (13, 92), linalool (132), and benzeneacetaldehyde (113). Group 2 showed higher

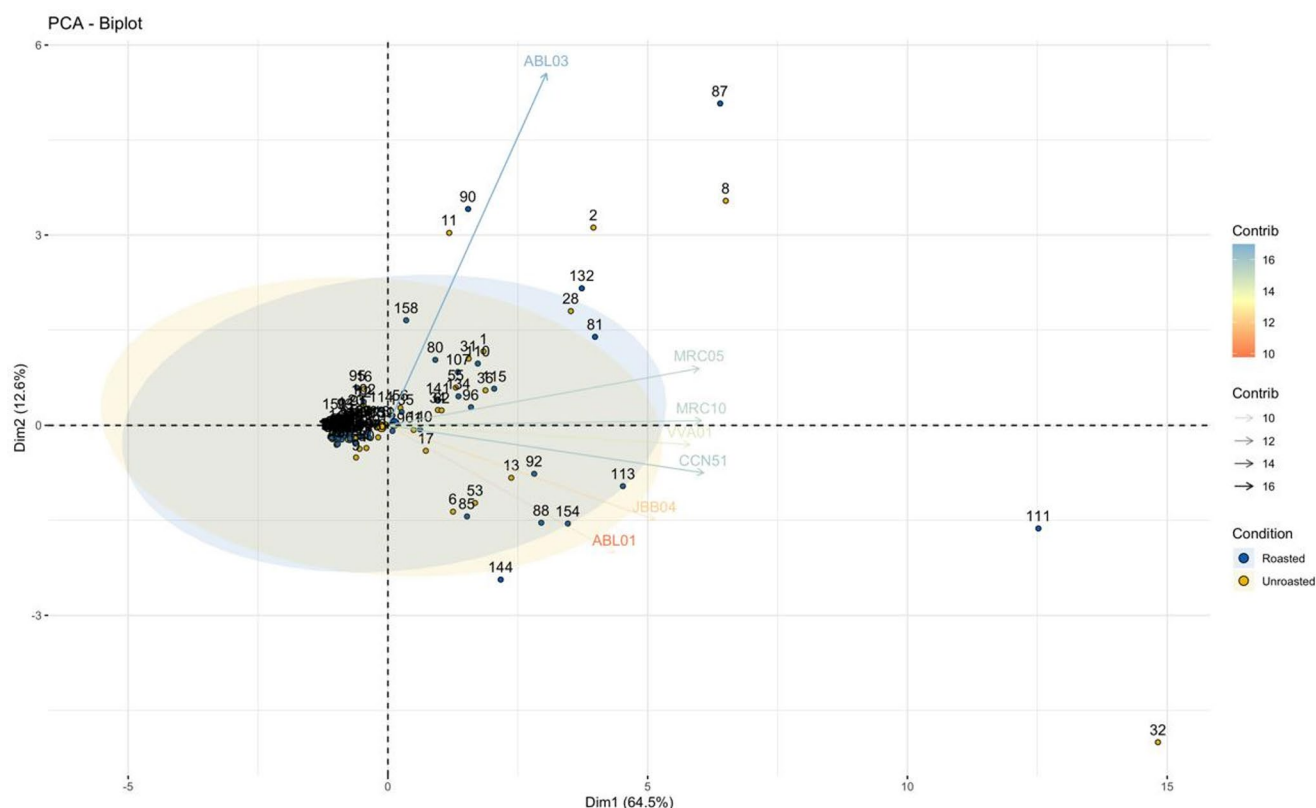


Fig. 1 Biplot for VOC and genotypes of unroasted and roasted cocoa beans. VOC is represented by numeric codes and the chemical names and other details can be found in Supplementary material. The codes for Unroasted samples range from 1 to 79, and for Roasted samples from 80 to 158

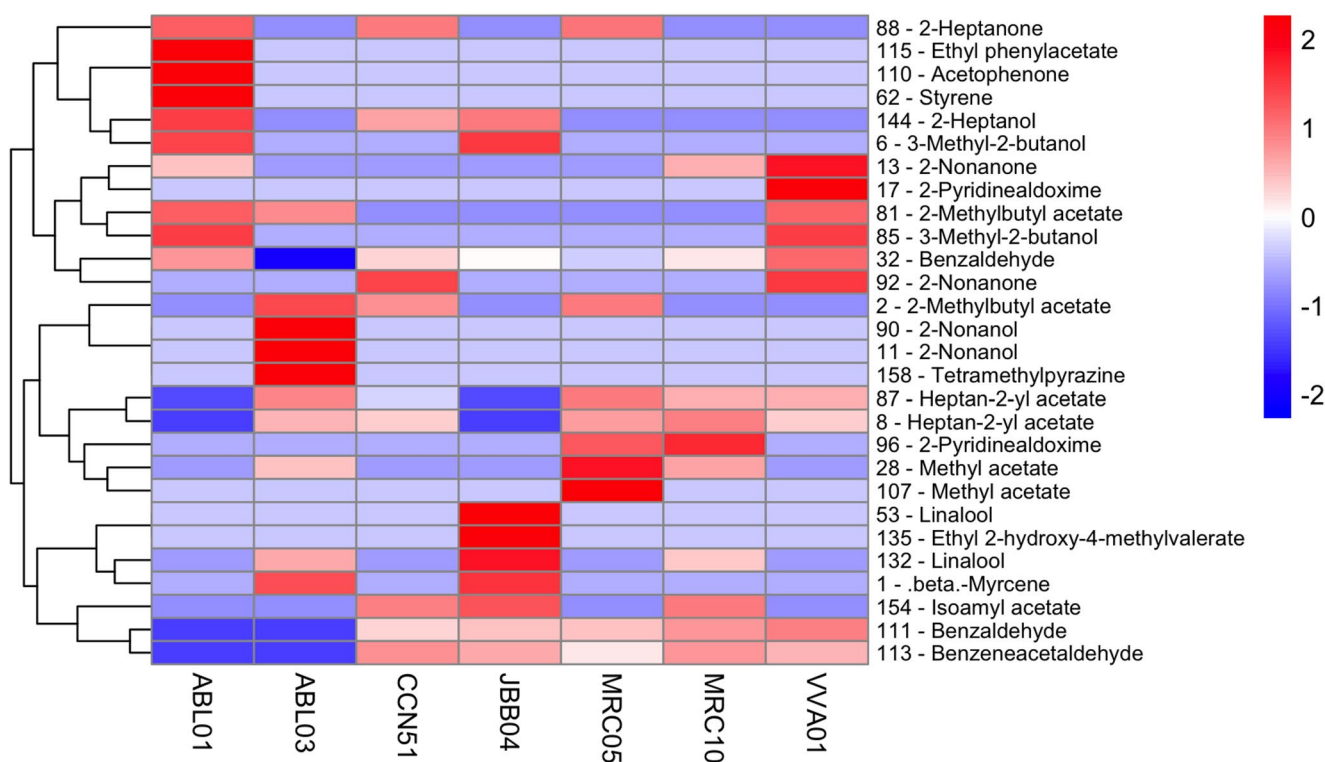


Fig. 2 Heatmap of key VOC by genotypes with the number code and the VOC name

contributions from heptan-2-yl acetate (8, 87), 2-nonanol (11, 90), linalool (132), 2-methylbutyl acetate (2, 81), tetramethylpyrazine (158), and methyl acetate (28). Group 3 was characterized by the presence of benzaldehyde (32), 2-heptanol (144), 2-heptanone (88), 2-nonanone (13), ethyl phenylacetate (115), and 3-methyl-2-butanol (6, 85). Group 4 showed major contributions from benzaldehyde (32, 111), linalool (53, 132), isoamyl acetate (154), benzeneacetaldehyde (113), and ethyl 2-hydroxy-4-methylvalerate (135).

Figure 2 provides a heatmap representation of these VOC highlighting their distribution and correlation across genotypes. Clustering was performed using Euclidean distance and complete linkage, allowing for the identification of patterns of similarity and differentiation among genotypes. The darker color intensities in the heatmap represent higher normalized contributions of VOC, facilitating visual identification of dominant compounds within each genotype.

Discussion

During fermentation, the protein content decreases, reaching values between 11.5 and 13.9%, which may be due to the degradation of globulins by the action of peptidases. In addition to reducing sugars, free hydrophobic peptides and amino acids are the precursors of the specific cocoa aroma [21]. The protein content of 14.51% found for the CCN51

genotype coincides with Perea et al. [22]. Lares-Amaíz et al. [23] studied the physicochemical properties of cocoa beans from Venezuela, obtaining 12.21% protein for sun-dried fermented beans. However, Hashimoto et al. [24] performed a quality control of commercial cocoa beans and found protein values between 13.8 and 16.0%. Overfermentation could be related to the low protein, which is associated with cocoa quality [25] and may lead to undesirable changes, such as the development of off-flavours and alterations in the balance of volatile organic compounds (VOC) [26]. However, not all genotypes that were over-fermented (fermentation index greater than 1.6) presented low protein percentages. There seems to be a greater relationship between total phenolic compounds and fermentation index, being that out of four over-fermented genotypes, three of them presented the lowest contents of total phenolic compounds. During fermentation, polyphenols decrease because they diffuse out of the beans, degrade and react with other compounds [27, 28].

Fat content is an important and most valuable quality index that influences the marketing of cocoa beans [15], mainly due to the rheological and textural characteristics that it can confer to chocolate [29]. The determination of this parameter and the search for varieties that offer higher lipid content is very interesting for the cocoa industry [30]. However, there are reports in the literature of low-fat percentages in fine aroma cocoa. Vera-Chang et al. [31] evaluated the fat content of fifteen cocoa clones in Ecuador,

obtaining a general average of 30.82% fat. This result is like that obtained in our research, with the highest fat content of 29.54% in ABL01 while CCN51 had 27.12% fat. However, it differs from that described by Álvarez et al. [32], who found an average crude fat yield of 53–56%, depending on the variety. Fat content can be affected by genetic factors, such as the extraction time [33] or the degree of fermentation of the beans, since the fat extraction yield in unfermented beans is higher than in beans with partial or complete fermentation [34]. Another factor that could affect is the manual grinding, which may explain the low-fat results due to the difficulty in obtaining small particles, considering that the smaller the particle size, the greater the extraction of fat content [12].

The ash percentages of the CCN51 and VVA01 genotypes were like those found for national cocoa clones, with a range between 2.55 and 4.04% ash [31]. On the other hand, Perea et al. [22] mention that the ash percentage should be between 3.2 and 3.9% to be considered premium fine cocoa. The ash content decreases during the fermentation process and long storage times of the pods are processes that also decrease the protein and total fat percentages while increasing the carbohydrate content [15]. For the latter, the lowest value was for the ABL01 genotype and the highest for JBB04, when compared to CCN51, which obtained a carbohydrate percentage of $50.55\% \pm 3.08\%$ and the lowest ash percentage ($2.14\% \pm 0.01\%$).

During the drying process, moisture is reduced from 60 to 8% and the slow loss of moisture favors the volatilization of acetic acid, preventing the pH from reaching values lower than 4 due to the loss of this organic acid [35]. The pH results found indicate that the cocoa was well processed, since values close to 5 were obtained [36], which lead to an increase in the aromatic potential of cocoa, whereas low pH levels (≤ 4.5) decrease this potential [37]. Acidification and the increase in temperature during fermentation influence the development of the flavour of the cocoa beans, as well as on the quality of the final product made with this raw material [38]. A pH between 4.75 and 5.19 indicates good fermentation and implies good conditions for the efficient action of enzymes that degrade bean protein and favour the generation of aroma and flavour precursors [39]. However, high pH values may indicate poor bean fermentation [40], as in the case of the above-mentioned genotypes (MRC05, VVA01, CCN51, and ABL01) with pH values between 5.3 and 5.4.

The highest values of fermentation index were found in ABL01 with 2.10 ± 0.04 and MRC05 with 2.57 ± 0.06 , which, together with the pH results and phenolic compounds, show possible problems in fermentation. It is important to consider that the storage time (under freezing) of the beans in the laboratory, between collection and analysis, varied from

8 to 15 months, and could have influenced the high indices found. Likewise, these fermentation indices may have been influenced by different fermentation conditions, since this procedure was not necessarily carried out simultaneously for each genotype in the cooperative. This last possibility seems more probable. CCN51 cocoa beans are fermented separately from the rest of the Criollo genotypes when the producers arrive at the agricultural cooperative (personal observation). This represents one of the main limitations of the study. Experiments conducted under controlled fermentation conditions will help to verify our results.

Phenolic compounds contribute to sensory quality, since their high content is associated with bitterness and astringency in the chocolate industry [24], in addition to imparting the characteristic reddish-brown color of cocoa and its derivatives [41], which is more representative in CCN51. The content of phenolic compounds found was like that reported by Efraim et al. [17] who found values between 61.0 and 215.5 mg TAE/g of nine cocoa genotypes. It is important to note that environmental factors, including agricultural practices, can affect the chemical composition of cocoa beans, including their phenolic compound content [17]. The high content of phenolic compounds plays an important role in bioactivity and has a beneficial effect on health [9]. However, very high levels can affect the sensory quality of the products obtained, since they decrease the formation of pyrazines [42], which are responsible for the formation of the characteristic flavours and aromas of chocolate and, therefore, if decreased, they reduce the quality of the chocolate. This effect was observed in the genotypes JBB04 and CCN51, which showed high levels of phenolic compounds and low abundance of VOC classified as pyrazines. However, the genotype ABL03 that have the greatest influence of tetramethylpyrazine (158), exhibited intermediate levels of phenolic compounds.

The aroma of cocoa is unique and there is no specific compound that determines this characteristic. Both volatile and non-volatile compounds are formed during chemical, physical and biological changes, conferring specific and important characteristics to the aroma of cocoa and, consequently, of chocolate [43]. Our discussion about aroma is based in literature review and it has not been estimated in this study.

In the present work, a total of 79 volatile organic compounds (VOCs) were identified. Of these, 68 were found in at least one genotype of roasted cocoa beans, and 64 in unroasted beans. The number of VOCs detected per genotype ranged from 36 (ABL03) to 44 (MRC05) in unroasted beans, and from 41 (ABL03) to 54 (CCN51) in roasted beans. These compounds included 2 acids, 10 alcohols, 7 aldehydes, 30 esters, 1 furan, 3 hydrocarbons, 5 ketones, 2 lactones, 1 phenol, 1 pyran, 5 pyrazines, 4 terpenes, and

8 other miscellaneous compounds. Several VOCs were found exclusively in roasted beans, such as the acids (benzoic acid and lactic acid), alcohols (2-heptanol and linalool oxide), aldehyde (decanal), esters (e.g., isoamyl acetate, octyl acetate), one furan (2-pentylfuran), one pyran, two pyrazines, and others. Conversely, a few compounds were detected only in unroasted beans, including alcohols, esters, hydrocarbons, one lactone, and other volatiles. This broad diversity reflects the complex nature of cocoa aroma and underscores the influence of both genotype and processing steps on the VOC profile.

Ten alcohols were identified in unroasted and roasted cocoa beans. Among them, 3-methyl-2-butanol (6, 85), a secondary amyl alcohol formed through sugar degradation during fermentation [44], showed higher abundance in unroasted ABL01 and JBB04 compared to MRC05 and MRC10, and was also more prominent in roasted ABL01 and VVA01 than in CCN51, JBB04 and MRC10. This compound had a high contribution in roasted ABL01 and VVA01 (Fig. 2). 2-Heptanol (144) has a strong contribution in roasted beans of the ABL01 genotype. Even though this compound was also identified in roasted JBB04 and CCN51, it contributes to the fruity aroma of cocoa, even at low concentrations [38, 45]. Linalool, a terpene with an alcohol functional group, is one of the key compounds responsible for the fine aroma of cocoa [38]. It is a biosynthesis product primarily associated with the fermentation process and influenced by plant variety, cultivation, and fermentation conditions [13]. Although, linalool (53, 132), a terpene alcohol, showed a high contribution in both unroasted and roasted beans of genotype JBB04, and a moderate contribution in roasted genotypes ABL03 and MRC10, its content is known to decrease during roasting due to volatilization. However, this expected reduction was not observed in our results.

Aldehydes and pyrazines are the main compounds formed during roasting [46, 47]. In this study, tetramethylpyrazine was detected only in roasted beans of the ABL01, ABL03 and VVA01 genotypes. Nevertheless, it contributed significantly only to ABL03 (Fig. 2) among the cocoa genotype groups identified in Fig. 1. In more recent works it was shown that pyrazines, in general, can be formed not only during roasting, but also during fermentation due to enzymatic reactions [48, 46], corroborating the presence of this group of compounds in the unroasted beans of the present work. Trimethylpyrazine can confer earthy, musty, potato and roasted smell, and 2,3-dimethylpyrazine, provides caramel, cocoa, hazelnut, peanut butter and roasted smells. Some authors indicate the use of high drying temperatures, besides increasing energy consumption and processing costs, can lead to a decrease in the concentration of desirable compounds such as tetramethylpyrazine, while

promoting the formation of undesirable compounds such as guaiacol, phenol, and certain acids [49]. Among the genotypes analyzed, MRC10 was the only one in which guaiacol (58, 137) was detected in both unroasted and roasted cocoa. In contrast, guaiacol was found at low relative abundance in genotypes CCN51, ABL01, JBB04, and MRC05. Figures 1 and 2 does not show a strong contribution of these undesirable compounds in the mentioned genotypes, as they are near the origin of the biplot (data not shown).

Aldehydes are common aromatic components of natural products and are widely used as food flavourings. Their presence can reflect the degree of cocoa roasting [46] and, together with ketones, enhance cocoa quality by contributing fruity and floral notes [50]. A lower concentration of fatty acids in the beans may be associated with a higher abundance of long-chain lipophilic compounds, such as aldehydes and esters [51]. This profile, characterized by low fat content and elevated levels of aldehydes and esters-is a distinctive feature of fine aroma cocoa. The benzaldehyde (32, 111) has a moderate contribution in roasted CCN51, JBB04, MRC05, MRC10, VVA01 genotypes, and unroasted CCN51, ABL01, and VVA01 genotypes. Previous findings indicate benzaldehyde as one of the major odor compounds in cocoa powder, irrespective of its geographical origin [50]. However, benzeneacetaldehyde (34, 113) also significantly influence cocoa's aroma, evaluating the total chemical composition rather than focusing solely on individual compounds may provide a more accurate representation of cocoa's sensory profile.

Bonvehí [50] reported higher concentrations of acetophenone in roasted cocoa beans, a compound associated with floral and sweet aroma notes [49]. In the present study, this effect was confirmed by the increased abundance of acetophenone (31, 110) in roasted beans. As shown in Fig. 2, this compound exhibited a particularly high contribution in the roasted ABL01 genotype. Other ketones presented in Fig. 2, such as 2-heptanone and 2-nonanone, may also contribute to the cocoa flavour by imparting fruity and floral notes [52].

Esters are part of the most abundant group of compounds in all the genotypes studied and are of great importance for the flavour of natural products [46]. These compounds are associated with fruit and floral notes and represent the second most important group of volatiles after pyrazines. Yeasts, during fermentation, are key producers of esters, especially in the early stages, as they condense acetyl-CoA with ethanol or other higher alcohols to form esters [38]. In general, esters are found more frequently and abundantly in fermented cocoa beans [53]. Likewise, their concentration can increase during roasting, particularly in cases of over-roasting [46]. In this study, several esters were detected and may contribute to the aroma profile of specific genotypes. Notably, the contributions of isoamyl acetate (75, 154),

heptan-2-yl acetate (8, 87), 2-methylbutyl acetate (2, 81), and ethyl phenylacetate (36, 115) to different genotypes are illustrated in Fig. 2.

Different genotypes or hybrids may present differences in the fermentation dynamics, requiring further research into individualized post-harvest processes that take into consideration the physical and chemical characteristics of cocoa [54]. Such processes may favor the development of certain microbial communities, generating physicochemical changes during cocoa fermentation [55].

This study reinforces the notion that fine aroma cocoa populations are genetically heterogeneous. The decision to establish plantations using single genotypes with desirable traits or heterogeneous populations with potentially greater resilience—but possibly lower productivity or increased challenges in product standardization—should be based on multiple factors. Despite the limitations of the present research, the results also appear to support the widely accepted understanding that postharvest processing steps, such as roasting, have a strong influence on the characteristics of the final product, potentially overriding or competing with the specific effects of genotype—at least at the level of volatile organic compounds (VOCs).

Conclusions

The results obtained in this study highlight the chemical and volatile diversity among the cocoa genotypes analyzed, reflecting both genetic variability and differences in post-harvest conditions. Significant differences were observed in protein, fat, ash, and carbohydrate contents, while the number and type of VOC—particularly esters, aldehydes, pyrazines, and ketones—varied notably between genotypes and between roasted and unroasted beans. Some genotypes, such as ABL01 and ABL03, exhibited a stronger presence of desirable aroma compounds like tetramethylpyrazine, acetophenone, and linalool, while others showed possible fermentation issues based on high fermentation indices, altered pH, or reduced protein content. These findings underscore the need for optimized and genotype-specific postharvest processing, especially fermentation and roasting, to ensure flavour quality in fine aroma cocoa. The comprehensive characterization of VOC profiles contributes to the selection and valorization of elite genotypes, providing a foundation for future research and strategies aimed at improving cocoa quality and premium chocolate production.

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Data availability No datasets were generated or analysed during the current study.

Declarations

Competing interests The authors declare no competing interests.

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