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Genetic-environment interactions and climatic variables effect on bean physical characteristics and chemical composition of *Coffea arabica*

Thuan Sarzynski^{1,2,3}, Benoît Bertrand^{1,2}, Clément Rigal^{4,5,6}, Pierre Marraccini^{1,2,7}, Philippe Vaast^{6,8}, Frédéric Georget^{1,2}, Claudine Campa^{2,9}, Cécile Abdallah^{2,9}, Chang Thi Quynh Nguyen³, Hung Phi Nguyen³, Hai Thi Thanh Nguyen^{3,10}, Quyen Luu Ngoc¹⁰, Giang Khong Ngan⁷, Thang Vu Viet¹¹, Luciano Navarini¹², Valentina Lonzarich¹², Laurent Bossolasco¹³, Hervé Etienne^{1,2}.

¹ CIRAD (Centre de Coopération Internationale en Recherche Agronomique Pour le Développement), UMR DIADE, F-34398 Montpellier, France.

² UMR DIADE (Diversity, Adaptation, Development of Plants), University of Montpellier, CIRAD, IRD, F-34398 Montpellier, France.

³ NOMAFSI (Northern Mountainous Agriculture Forestry Science Institute) Mai Son research centre, Son La, Vietnam

⁴ CIRAD UMR ABSYS, Montpellier, France.

⁵ ABSYS, Université Montpellier, CIRAD, INRAE, Supagro, Montpellier, France.

⁶ ICRAF, Vietnam office, Hanoi, Vietnam.

⁷ AGI (Agriculture Genetics Institute), Hanoi, Vietnam

⁸ UMR Eco & Sols, CIRAD, 34398 Montpellier, France

⁹ IRD (Institut de Recherche pour le Développement), Montpellier, France

¹⁰ NOMAFSI headquarter, Phu Tho, Vietnam

¹¹ Phuc Sinh Son la corporation, Son La, Vietnam

¹² illycaffè S.p.A., via Flavia 110, I-34147 Trieste, Italy

¹³ ECOM-SMS (Sustainable management services ECOM Agroindustrial), Ho Chi Minh City, Vietnam

*correspondence to Thuan Sarzynski, thuan.sarzynski@cirad.fr

Abstract

BACKGROUND

The effects of the environment and genotype in the coffee bean chemical composition were studied using 9 trials covering an altitudinal gradient (600 – 1100 m.a.s.l) with 3 genotypes of *Coffea arabica* in the Northwest mountainous region of Vietnam. The impacts of the climatic conditions on bean physical characteristics and chemical composition were assessed.

RESULTS

We showed that the environment had a significant effect on the bean density and on all bean chemical compounds. The environment effect was stronger than the genotype and genotype-environment

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interaction effects for cafestol, kahweol, arachidic (C20:0), behenic acid (C22:0), 2,3-butanediol, 2-methyl-2-buten-1-ol, benzaldehyde, benzene ethanol, butyrolactone, decane, dodecane, ethanol, pentanoic acid, and phenylacetaldehyde bean content. A 2°C increase in temperature had more influence on bean chemical compounds than a 100 mm increase in soil water content. Temperature was positively correlated with lipids and volatile compounds. With an innovative method using iterative moving averages, we showed that correlation of temperature, VPD and rainfall with lipids and volatiles was higher between the 10th and 20th weeks after flowering highlighting this period as crucial for the synthesis of these chemicals. Genotype specific responses were evidenced and could be considered in future breeding programs to maintain coffee beverage quality in the midst of climate change.

CONCLUSION

This first study of the effect of the genotype-environment interactions on chemical compounds enhances our understanding of the sensitivity of coffee quality to genotype environment interactions during bean development. This work addresses the growing concern of the effect of climate change on speciality crops and more specifically coffee.

Keywords : coffee ; bean chemical content ; genetic-environment interactions ; climate change

INTRODUCTION

Each stakeholder of the coffee value chain has its own definition of coffee quality. While bean size, defects and origin are important for coffee traders and roasters, ultimately the consumer experiences and judges coffee sensory quality notably through its aroma and flavour ¹. The coffee sensory quality has been linked to the compounds identified in green coffee beans; for example, fatty acids have been correlated with better beverage aroma, and trigonelline with stronger bitterness ^{2,3}. Among the compounds identified in mature coffee beans, those presented in high amounts on a dry matter basis are lipids ($\pm 150 \text{ g}\cdot\text{kg}^{-1}$) ⁴, proteins ($\pm 100 \text{ g}\cdot\text{kg}^{-1}$) ⁵ and sucrose ($\pm 100 \text{ g}\cdot\text{kg}^{-1}$) ⁶. Phenols like chlorogenic acids ($\pm 60 \text{ g}\cdot\text{kg}^{-1}$) as well as alkaloids like caffeine ($\pm 20 \text{ g}\cdot\text{kg}^{-1}$) and trigonelline ($\pm 20 \text{ g}\cdot\text{kg}^{-1}$) ^{7,8} were reported as important compounds of coffee cup quality ^{9,10}. Volatile compounds ($< 10 \text{ g}\cdot\text{kg}^{-1}$) have been linked to flavour defects in coffee ^{11,12}, despite being associated with high sensory quality in other beverages ^{13,14}.

Studies on *Coffea arabica* (60% of the global coffee market) have reported that bean chemical compounds and therefore coffee sensory quality are in turned impacted by environmental conditions ^{3,15-19}. For example, temperature was reported to have more effect on bean content and chemical composition than any other environmental variable ^{18,20,21}, with high temperature linked with low bean weight and density, and high bean content of chlorogenic acids, alkaloids, and fatty acids ²². Soil water availability and irrigation were also found to increase bean size, yield, as well as phenols, lipids, chlorogenic acid bean content, and cup quality ^{20,23-25}. Altitude and shade have been found to increase bean size and density ^{26,27} as well as bean fatty acids ²⁸. The coffee growing environment also influenced volatile compounds and contributed to define trade classifications based on geographic origin ^{29,30}. Similar results were found with other crops, highlighting strong links between environmental conditions and crop chemical quality ³¹.

Coffee bean chemical compounds and quality also depend on genetic factors. For example, varieties of *C. arabica* recently introgressed with *C. canephora* genes were found to differ in bean caffeine, chlorogenic acids, fat, and sucrose bean contents ³². This opens opportunities to breed genotypes with better quality ^{1,33,34}. The genetic diversity of *C. arabica* introduced in Vietnam is very low with the variety 'Catimor' alone representing more than 95% of the orchard. Bringing genetic diversity with new elite *C. arabica* genotypes with better agronomic performances can prevent future pest epidemics and improve the commercial prospect of Vietnamese coffee in the global market.

Finally, the genetic-environment interactions (GxE) also impact chemical composition and the resulting coffee quality. Bean content of *C. arabica* was shown to respond differently to elevation depending on

the genotype, elevation increased fat content in commercial lines but stayed constant for F1-hybrids resulting from the cross between wild Ethiopians and commercial lines, it was also less correlated with chlorogenic acids for the lines than for the F1-hybrids¹⁵. These F1-hybrids developed in the last decades have shown better bean physical characteristics and better sensory quality^{19,35,36}.

Climate change across the globe is predicted to decrease the area suitable for coffee plantation and to create new frontiers for coffee establishment^{37,38}, however the effects of climate change on the quality of coffee in these frontier areas with suboptimal conditions are not well studied. The Northwest of Vietnam presents suboptimal conditions for cropping *C. arabica* as it is situated at the latitudinal limit of the tropical belt. In this particular geo-climatic location, can small changes in climatic conditions and in genotypes modify essential determinants of green coffee quality?

The present study assesses the genetic-environment interactions as well as the effects of specific climatic variables on green coffee bean physical characteristics (bean density, size and defects) and chemical composition (phenols, alkaloids, terpenes, fatty acids, and volatile compounds) for 3 *C. arabica* genotypes. This study also highlights the effect of temperature during the different bean development stages on bean biochemical content.

MATERIALS AND METHODS

Plant Material

Three *C. arabica* genotypes were used: two fixed lines (the local Catimor, used as control, and Marsellese) and one F1-hybrid (Starmaya). Catimor (C) and Marsellese (M) respectively originated from crosses between Timor Hybrid 832/1 x Caturra and Timor Hybrid 832/2 x Villa Sarchi CIFC 971/10, respectively. Starmaya (HS) resulted from a cross between the sterile male CIR-SM01 and Marsellese and can be propagated by seeds^{36,39}.

Seeds of M and HS were provided by ECOM-Nicaragua in the framework of the BREEDCAFS project. Seeds of the local C were collected (Nov. 2017) from a unique plant available in the coffee germplasm of NOMAFSI (Northern Mountainous Agriculture and Forestry Science Institute) research station in Mai Son district, Son La province. All seeds were germinated and grown (from Nov. 2017 to April 2018) in Agriculture Genetics Institute (AGI, Hanoi). Plantlets with a similar development were later transferred to NOMAFSI nursery for a 2-month additional growth period to reach a 30-cm size before being planted on farmers' field in July 2018 (rainy season).

Location and experimental design

The study was carried out in Son La and Dien Bien mountainous provinces (annual average temperature $\pm 22^{\circ}\text{C}$, annual rainfall ± 1500 mm) of North-West Vietnam (Fig. 1A) where the climate has low rainfall and high seasonal and daily temperature changes (SM Figure 3). The elevation spans from 600 to 1100 m.a.s.l with steep slopes. Coffee plantations are usually established on sloping lands and unshaded conditions (Fig. 1F). For our study, 9 trials were established in areas with contrasting environmental conditions (Fig. 1, Table 1).

Each trial was organized in a random block design with 8 plots with 50 coffee trees each and a plant spacing of 2 m between rows and 1.5 m within rows (Fig. 1C). Each genotype was planted in 2 plots and the local Catimor (C) was used in the borders separating plots (2 rows) and surrounding the trial. Even though recommendations on management were provided to each farmer based on the soil analysis of their farm (data not shown), farmers were free to manage their plantation based on their skills and financial capacities. Nonetheless, all genotypes received the same management in each trial.

Figure 1. Design and location of the trials studied in the North-West of Vietnam. (A) Global map locating Vietnam in Southeast Asia. (B) Location of the 9 trials (block dots) in Son La and Dien Bien provinces. (C) Design of trial n°8, each coloured square represents a plot with a *C. arabica* genotype: Catimor (black), Starmaya (red), Marsellese (white). Yellow squares included genotypes not studied here.

Environmental monitoring

Environmental conditions were monitored for each trial from the March 15th to Nov. 30th 2020, corresponding to the period between coffee flowering and the last harvest peaks. Nine environmental factors were monitored: average (Tavg), minimum (Tmin) and maximum (Tmax) temperatures, average (VPDavg) and maximum (VPDmax) vapor pressure deficit, soil humidity of the first 50 cm (SH50) and the first 100 cm (SH100), rainfall (RF), and solar radiation (SR). The air temperature and humidity were recorded every hour using a Hygrochron Temperature and Humidity iButton (DS1923-F5; Embedded data systems, USA). Tavg was calculated by averaging the daily average temperature from the peak of flowering to the peak of harvest. Tmin, Tmax were calculated by averaging the daily minimum and maximum temperature of the same period, respectively.

The VPD was calculated with the temperature and humidity following Equation 1 below:

$$VPD = \frac{H}{100} * \frac{610.7 * 10^{\frac{7.5T}{237.3+T}}}{1000} \quad (1)$$

where T is air temperature and H is air humidity. The VPDavg was calculated by averaging the daily average VPD while the VPDmax corresponds to the average of daily maximum VPD measured during the same period. For each trial, soil humidity was measured with a Diviner 2000 probe (Sentek Technologies, Australia) every 10 cm between the soil surface and down to 1-m depth in 2-3 access tubes per trial. Measurements were taken once at the end of the dry season (May). Data from all the tubes on a same trial were averaged to get an overall soil water content of that trial. Soil humidity between 0 and 50 cm were summed up to obtain an average soil humidity of the first 50 cm (SH50) and the first 100 cm (SH100).

RF data were bought from Watec (<https://www.watec.vn>). The 5 weather stations from which data were retrieved were located less than 10 km from the trials. Daily rainfall data were summed to obtain the total rainfall over the studied period. SR was retrieved from an online solar data provider named Solcast (<https://solcast.com/>). The Solcast data company provides datasets of solar irradiance at a 2 km spatial resolution based on the imagery of 3 weather satellites, namely, Himawari 8, GOES-16, GOES-17 and the clear-sky model, REST2v5^{40,41}. The monthly SR were summed up to obtain an estimation of the total solar irradiance of the studied period.

Table 1. Environmental variables in each of the 9 trials.

N°	Province	EL	Tavg	Tmin	Tmax	VPDavg	VPDmax	SH50	SH100	RF	SR
1	Dien Bien	638	24.2	20.3	30.8	0.75	2.04	221	461	1960	1100
2	Son La	716	23.2	18.7	30.6	0.49	1.87	189	377	1290	1110
3	Son La	729	23.7	19.2	31	0.6	2.04	167	327	1290	1110
4	Son La	744	23.6	18.8	31.1	0.6	2.06	207	444	1030	1140
5	Son La	745	23.6	19.2	30.9	0.56	1.96	197	347	1030	1140
6	Son La	794	24.8	20	33.4	0.9	2.87	217	471	1180	1120
7	Son La	829	23.4	18.5	31.6	0.62	2.37	158	342	1180	1100
8	Dien Bien	1020	22.1	18.6	27.5	0.53	1.5	205	445	1460	1080
9	Dien Bien	1070	22.3	18.7	27.9	0.42	1.23	248	499	1460	1080

Parameters analysed: elevation (EL, in meter above sea level m.a.s.l), temperatures (°C) corresponding to average (Tavg), minimum (Tmin) and maximum (Tmax), VPD (kPa) corresponding to average (VPDavg) and the maximum (VPDmax), soil humidity (SH50 and SH100 expressed in mm H₂O), Rainfall (RF, mm H₂O), and solar radiation (SR, kWh m⁻²).

Harvest and post-harvest processes

Accepted Article

Trials were harvested in 3 to 5 times between Oct. and Nov. 2020 on 2.5-year-old trees, it was the first real harvest. For each genotype in each trial, one sample of cherries was collected at the peak of ripeness. Cherries were washed in water two times (NOMAFSI research station). Floating and defective cherries were then weighted and discarded. Healthy cherries were pulped in a small mill. Beans were fermented in water in a 220-L bucket for 15-19 h (HoursFe) and washed thoroughly before being sundried for 14-17 days (DaysDr, DateDr) until they reached a humidity of 12% (SM Figure 1). The average air temperature during the wet fermentation (TavgFe) and the bean drying (TavgDr) were monitored with the weather station of the NOMAFSI centre (SM Table 1). All these data are in supplementary materials. Dried beans were shipped to the different partners for bean grading, and bean chemical composition analysis.

Degree days

Degree days is an indicator of the heat accumulated by the plant over a period of time. A base temperature of 10°C was used as a bottom threshold under which coffee plants do not photosynthesize⁴². The number of days before harvest and the degree days were calculated based on trials only, without differences between genotypes (SM Table 1). The number of days (N-days) between flowering (PeakFl) and harvest (DateH) were calculated by subtracting PeakFl to DateH. Degree days (D_{day}) between PeakFl and DateH were calculated as in Equation 2 below:

$$D_{day} = \sum_{PeakFl}^{DateH} (T_{avg} - 10) \quad (2)$$

With D_{day}, the degree days, DateH, the date of harvest, PeakFl, the peak of flowering, T_{avg}, average temperature.

Physical characteristics of coffee beans

After harvest of the trials and post-harvest processing of all the samples, 300-g of dried beans were used to evaluate bean sizes, using a sieve with round perforations of diameter 6.3 mm for Grade 16 and 7.1 mm for Grade 18. These two grades were weighted together to obtain the exportable beans (Grades 16 + 18), the standard size of traded green coffee beans. Defects were removed to prepare green bean prior roasting. The bean density in kg.m⁻³ was measured by filling a given volume with green beans and weighting the beans.

Biochemical analysis

All biochemical analysis were carried out on green beans of high grade (>16) harvested in one time at the peak of ripeness.

Alkaloid and phenolic compounds, namely trigonelline, caffeine, monocaffeoylquinic acids (3-, 4-, 5-CQA), dicaffeoylquinic acids (3,4-, 3,5-, 4,5-diCQA), coumaroylquinic acid (5-pCoQA), feruloylquinic acids (FQA) and catechin, were extracted by stirring (6 xg, Rotamax 120, Heidolph, Schwabach, Germany) 25 mg of green bean powder in 6 ml of methanol (MeOH)/H₂O (80:20, v/v). Compounds were quantified with a HPLC system (Shimadzu LC-20, Tokyo, Japan) at flow rate of 0.6 ml/min using Eclipse XDB C18 (3.5 μm) column (100 mm x 4.6 mm, Agilent) and an elution system made of solvents B (H₂O/MeOH/acetic acid, 5:90:5 v/v/v) and A (water/acetic acid, 98:2, v/v) as previously described¹⁹. Quantification of chlorogenic acids was undertaken at 320 nm, caffeine and catechin at 280 nm, trigonelline at 260 nm. Concentrations were determined based on standard curves generated from pure standard solutions (Sigma Aldrich, St Quentin, France) and expressed in mg·kg⁻¹ or g·kg⁻¹ of dry matter. Diterpenes, namely cafestol and kahweol were analysed with NMR spectroscopy using Bruker DMX600 spectrometer equipped with a 5mm TXI triple gradient probe (Bruker BioSpin, Rheinstetten; Germany). ¹H NMR spectra were collected using two Bruker Avance 400 MHz spectrometers running TopSpin 3.0 and 3.2 software, both equipped with a 5 mm BBI probe with Z-gradient coils and a SampleXpress autosampler (Bruker BioSpin, Rheinstetten; Germany). UPLC-MS/MS liquid, chromatography were performed with an Agilent 1290 UPLC interfaced to a SCIEX Triple Quad™ 4500, using a chromatography column Waters ACQUITY HSS T3 C18 (2.1 x 100 mm, particle size 1.8 μm) maintained at 30°C with a flow of 500 μL/min. A two solvent system was used: solvent A, 0.1% formic

acid in water; solvent B, acetonitrile; with an injection volume of 10 μ L and a linear gradient as follows: 0 min 40% A; 6.5 min 40% A; 9.5 min 20% A; 10 min 40% A. Cafestol and kawheol were quantified by integration of corresponding peaks, respectively, at 5.82 ppm, 6.14 ppm, and 3.10 ppm, using cafestol acetate as reference compound for response factor determination as previously reported ⁴³.

Fatty acids, namely myristic (C14:0), palmitic (C16:0), stearic (C18:0), oleic (C18:1), linoleic (C18:2), linolenic (18:3), arachidic (C20:0) and behenic (C22:0) acids were extracted from 20 mg of green bean powder and extracted with 2 ml of chloroform:methanol (1:1, v/v) and 1 ml H₂O and then 2 ml of chloroform. Fatty acid methyl esters were purified and detected using an Agilent 7890 gas chromatograph equipped with a DB-23 column (60 cm x 0.25 mm x 0.25 μ m, Agilent Technologies, Wilmington, DE) and flame ionization. Fatty acids were identified by comparing their retention time with commercial fatty acid standards (Sigma-Aldrich) and quantified using ChemStation (Agilent) to calculate the peak surfaces as previously described ^{43,44}.

Volatile compounds were extracted using a CAR/PDMS (carboxen/polydimethylsiloxane, 75 μ m) SPME fibre (Supelco Co., Bellefonte, PA, USA) and quantified by gas chromatography–mass spectroscopy (GC-MS) using a 6890A GC connected to a 5975B MS (Agilent, Palo Alto, USA) equipped with a 60 m ZB-WAX plus capillary column (film thickness: 0.25 μ m; internal diameter: 0.25 mm; Phenomenex, Bologna, Italy). Volatiles compounds were identified by comparing their calculated relative retention indexes with the literature, and their mass spectra with those available in the database (NIST11/Wiley10 libraries) as previously reported ¹⁹.

Statistical analyses

The effect of genotypes (G), environments (E) and their interactions (GxE) were assessed with a two-way ANOVA for the phenols (9 compounds), and alkaloids (2 compounds), terpenes (2 compounds), fatty acids (8 compounds), volatiles (27 compounds), and bean physical characteristics (5 variables). The percentage of variance attributable to each factor was calculated by dividing the sum of squares of each factor to the total, multiplied by 100, as previously described ⁴⁵.

The chemical compounds presenting environmental effects that were both significant and which explained most of the variation were investigated further with simple linear models against relevant environmental variables identified through a PCA. The significance of the correlation coefficients was assessed with a one-tailed t-test. The results of the simple linear models with the highest correlation coefficients were segregated by genotype to emphasize the genetic differences and their interaction with a specific climatic variable.

We created 14-time intervals between March 15th and Nov. 30th 2020, with a 15-day shift between consecutive intervals. Intervals covered 30 days each and thus overlapped. The average temperature, average VPD and cumulative rainfall were calculated for each of these 14 intervals. Rainfall was the only variable related to soil water content available with a daily resolution. Correlations were calculated between each of these 14 average temperatures, average VPD and cumulative rainfall with cafestol, kahweol, C20:0, C22:0, 2,3-butanediol, benzaldehyde, benzene ethanol, butyrolactone, pentanoic acid and phenylacetaldehyde, resulting in 14 correlation coefficients for each bean chemical compound. These compounds were chosen based on their high environment effect in the ANOVA and their high correlation with T_{avg} , VPD_{avg} and RF (Table 2, SM Table 2,3). The correlation coefficients were plotted against the time in weeks after flowering (WAF). This analysis was carried out on other bean chemical compounds and variables and the results are available in the supplementary materials (SM Table 4). All statistical analyses were performed on R Version 4.2.2 ⁵ ⁴⁶.

RESULTS

Bean chemical compounds and the effects of genotype, environment, and their interactions

Bean chemical compound contents obtained from the 3 genotypes and 9 trials are shown in Table 2 and detailed ANOVAs are in SM Table 5.

All bean chemical compounds as well as bean density were significantly influenced by G, E as well as GxE (Table 2). Other physical attributes - bean grades and bean defects - were neither significantly influenced by G, E, nor GxE.

The G effect was the highest for 3,4-diCQA, 4,5-diCQA, 5-pCoQA, FQA, catechin, 2-methoxy-3-isobutyl-pyrazine, 3-methyl-butanoic acid. The 3,4-diCQA, 4,5-diCQA, FQA, 3-methyl-butanoic acid and 2-methoxy-3-isobutyl-pyrazine had the highest concentration in C beans, while catechin and 5-pCoQA had the highest concentrations in those of M. The E effect was the highest for 3-CQA, 4-CQA, 3,5-diCQA, cafestol, kahweol, C20:0, C22:0, 2,3-butanediol, 2-methyl-2-buten-1-ol, benzaldehyde, benzene ethanol, butyrolactone, decane, dodecane, ethanol, hexanoic acid, pentanoic acid, phenylacetaldehyde, and toluene. The GxE effect was the highest for 5-CQA, trigonelline, caffeine, C14:0, C16:0, C18:0, C18:1, C18:2, C18:3, 1-hexanol, 1-pentanol, 2-methyl furan, 2-propanone, 2-methyl furan, acetic acid, benzyl alcohol, di-methyl sulphide, *d*-limonene, furfural, hexanal, pyridine, and all bean physical characteristics. Only the bean compounds for which the E effect was significant and higher than the G and GxE effects were kept for further analysis with PCA and correlations.

Table 2. Average, minimum and maximum values (avg, min, max) of the content of each compound in the coffee bean.

	Values			ANOVA		
	avg	min	max	G (n = 9)	E (n = 3)	G x E (n = 36)
Phenols						
3-CQA ^a (g·kg ⁻¹)	3.9	2.6	5.4	1***	61***	37***
5-CQA (g·kg ⁻¹)	34.8	23.9	40.2	11***	42***	47***
4-CQA ^a (g·kg ⁻¹)	5.5	3.7	6.7	1***	63***	36***
3,4-diCQA (g·kg ⁻¹)	1.6	1.1	2.4	47***	13***	41***
3,5-diCQA ^a (g·kg ⁻¹)	3.5	2.5	5.4	4***	59***	38***
4,5-diCQA (g·kg ⁻¹)	1.8	1.1	2.4	52***	14***	34***
5-pCoQA (g·kg ⁻¹)	0.6	0.4	0.9	44***	14***	42***
FQA (g·kg ⁻¹)	3.9	2.6	5.7	52***	6***	42***
catechin (g·kg ⁻¹)	0.7	0.5	1.0	49***	21***	31***
Alkaloids						
trigonelline (g·kg ⁻¹)	9.7	6.6	11.5	26***	26***	49***
caffeine (g·kg ⁻¹)	9.3	6.0	12.4	40***	12***	48***
Terpenes						
cafestol ^a (mg·kg ⁻¹)	3.9	0.7	9.1	24***	42***	34***
kahweol ^a (mg·kg ⁻¹)	4.1	0.4	6.6	12***	55***	33***
Fatty Acids						
C14:0 (mg·kg ⁻¹)	115.5	76.8	200.5	7***	31***	63***
C16:0 (mg·kg ⁻¹)	48359.8	36620.1	72836.9	11***	21***	68***
C18:0 (mg·kg ⁻¹)	10422.9	7048.6	12729.7	5***	47***	48***
C18:1 (mg·kg ⁻¹)	11267.6	5174.7	16930.5	14***	24***	62***
C18:2 (mg·kg ⁻¹)	50686.5	16723.9	74224.3	9***	32***	59***
C18:3 (mg·kg ⁻¹)	829.8	182.2	1330.4	12***	33***	56***
C20:0 ^a (mg·kg ⁻¹)	3523.9	2500.4	4525.8	6***	58***	36***
C22:0 ^a (mg·kg ⁻¹)	917.5	574.3	1355.1	2***	64***	33***
Volatile compounds						
1-hexanol (p.a)	607602.3	338147.3	842699.3	21***	24***	55***

1-pentanol (p.a)	94331.5	64579.0	124311.3	12***	26***	63***
2,3-butanediol ^a (p.a)	115750.4	14556.0	217046.3	4***	55***	41***
2-methoxy-3-isobutyl-pyrazine (p.a)	486750.2	270719.0	746532.0	50***	10***	40***
2-methyl furan (p.a)	202128.4	124365.3	290518.0	13***	42***	45***
2-methyl-2-buten-1-ol ^a (p.a)	69812.3	30883.7	210662.0	22***	51***	27***
2-propanone (p.a)	1066018.3	447331.7	1667395.3	5***	38***	57***
3-methyl butanal (p.a)	106225.4	45764.7	237277.0	36***	22***	42***
3-methyl furan (p.a)	169818.5	126712.0	225889.0	8***	14***	79***
3-methyl-butanoic acid (p.a)	189469.7	80551.7	373458.0	42***	38***	20***
acetic acid (p.a)	231672.1	107631.0	380761.0	33***	29***	38***
benzaldehyde ^a (p.a)	129305.0	90891.0	163456.0	2***	87***	11***
benzene ethanol ^a (p.a)	300979.8	186342.0	496250.7	9***	56***	35***
benzyl alcohol (p.a)	56360.7	37252.7	89598.0	16***	41***	43***
butyrolactone ^a (p.a)	133940.5	51739.0	243271.0	6***	54***	39***
decane ^a (p.a)	275285.6	205865.7	336367.0	22***	46***	32***
dimethyl sulfide (p.a)	86260.0	9579.7	659036.0	3***	45***	52***
dl-limonene (p.a)	742012.2	42206.7	2407405.7	41***	2***	57***
dodecane ^a (p.a)	373416.1	162555.3	568308.3	3***	64***	33***
ethanol ^a (p.a)	964999.4	442008.3	1688469.3	20***	57***	23***
furfural (p.a)	30097.7	13356.0	64993.0	1***	48***	51***
hexanal (p.a)	673444.6	394038.0	1006037.7	19***	29***	52***
hexanoic acid ^a (p.a)	148538.3	58843.7	297504.7	4***	52***	45***
pentanoic acid ^a (p.a)	148453.9	59663.3	297825.0	4***	52***	44***
phenylacetaldehyde ^a (p.a)	114950.2	71588.3	196152.7	4***	51***	45***
pyridine (p.a)	19051.2	0.0	122033.3	5***	41***	54***
toluene ^a (p.a)	77022.7	30708.7	195243.7	1***	63***	36***
Bean characteristics						
bean defects (%)	6.2	2.5	23.1	6	43	50
grade 18 (%)	42.5	3.4	76.2	2	43	55
grade 16 (%)	17.3	7.5	51.1	2	39	59
exportable beans (%)	80.2	55.5	94.8	11	33	56
bean density (%)	0.679	0.648	0.708	17***	36***	47***

Phenols and alkaloids are in g·kg⁻¹, terpenes and fatty acids are in mg·kg⁻¹, volatile compounds are in peak area (p.a), bean characteristics are in % (except for the bean density which is in kg·m⁻³). ANOVA of the differences between coffee genotype (G), environment (E), and their interactions (G × E) are displayed on the right side of the table. The percentage of variance explained by G, E and G×E is followed by the *p*-value of the ANOVA. Significance of *p*-values: 0 '***', 0.001 '**', 0.01 '*', 0.05 '.', 0.1 '.', and 1. Compounds for which E has the highest effect are indicated with (a). A total of 36 samples were included in the ANOVA, 9 per G and 3 per E.

Correlation of average environmental variables with bean chemical compounds

Environmental variables and bean chemical compounds were represented in two PCA to have an overview of their linear relationships. The variables representing the bean chemical compounds were included as supplementary variables in the PCA. The first dimension of the PCA on the horizontal axis is linked to air temperatures, with contributions from EL, Tavg, Tmin, Tmax, TR, VPDavg, VPDmax, SR and D-day, and explain 54.6% of the variability (Fig. 2, 3). That axis shows that Tavg, Tmin, Tmax,

TR, VPDavg, VPDmax, SR and D-day are all positively correlated together, and are all negatively correlated to EL (SM Fig. 2).

The second dimension is linked with soil water availability, with contributions from SH50, SH100 and RF, and explains 25.1% of the environmental data variability. SH50, SH100 and RF are positively correlated together. Among the bean content variables with a high and significant environment effect in the ANOVA, cafestol, kahweol, C20:0, C22:0, 2,3-butanediol, benzaldehyde, benzene ethanol, butyrolactone, dodecane, ethanol, hexanoic acid, pentanoic acid, phenylacetaldehyde had significant correlations with environmental variables of the first dimension of the PCA which are related to air temperature (Fig. 2, 3, SM Table 2,3). Moreover, 2,3-butanediol and dodecane correlated significantly with environmental variables of the second dimension of the PCA which are related with soil water availability. Among the bean content variables with a high and significant environment effect in the ANOVA, 3-CQA, 4-CQA, 3,5-diCQA, decane, 2-methyl-2-buten-1-ol, 3-methyl-butanoic acid did not show significant correlations with any environmental variable.

Correlation of the main environmental variables with bean chemical compounds segregated by genotypes

We chose to use Tavg and SH50 in the correlation analysis because they represented the first and second dimension of the PCA, respectively. The effects of Tavg and SH50 on bean chemical compounds presented some differences across the three *C. arabica* genotypes (Fig. 2, 3). Tavg correlated positively with the bean secondary metabolites like cafestol, C20:0 and C22:0 for all genotypes. However, C and M showed no correlation of Tavg with the bean content of kahweol. On the other hand, Tavg correlated positively with bean volatile compounds like ethanol, benzaldehyde, benzene ethanol, hexanoic acid, pentanoic acid, butyrolactone, phenylacetaldehyde, dodecane and negatively with 2,3-butanediol. In these cases, differences for some genotypes were also noticed. For example, M had no correlation of Tavg with hexanoic acid, pentanoic acid, phenylacetaldehyde and dodecane bean volatile compounds while C had no correlation of this variable with ethanol and benzene ethanol bean volatile compounds. No correlation of Tavg with dodecane, 2,3-butanediol and ethanol bean volatile compounds was observed (Fig. 3) and SH50 correlated positively with 2,3-butanediol, but negatively with dodecane bean volatile compounds for S. On the other hand, C showed no correlation of SH50 with 2,3-butanediol and dodecane.

Correlation of temperature, VPD and rainfall with different bean biochemical compounds at different stages of the bean development

Correlations of the volatile compounds, lipids and terpenes with Tavg were positive (except for 2,3-butanediol) with low coefficients in the first 4 weeks after flowering and the last four weeks before the harvest. Correlations were higher during stages of high Tavg; for example, between the 6th and 24th weeks after flowering (WAF) (Fig. 4: A1, A2). Correlations of the volatile compounds, lipids and terpenes with VPDavg were positive (except for 2,3-butanediol) and had high coefficients from the 6th to the 14th WAF. For benzene ethanol and butyrolactone, the coefficients were high on the 20th and 22nd WAF. For phenylacetaldehyde, correlation coefficients were significant only on the 8th WAF (Fig. 4: B1, B2).

Correlations of the volatile compounds, lipids and terpenes with rainfall were negative, except for 2,3-butanediol. The highest coefficients were on the 10th WAF, except for benzaldehyde which had the highest correlation coefficients on the 18th and 20th WAF. The correlation of the lipids and terpenes with the rainfall had the highest coefficients in the 14th and 16th WAF (Fig. 4: C1, C2, SM Table 4).

Figure 2. PCA and regression of climatic variables from 9 trials in the Northwest of Vietnam with secondary metabolites from the bean content of 3 genotypes: Catimor (C), Marsellea (M), and Starmaya (HS). EL (elevation), Tavg (average temperature), Tmin (minimum temperature), Tmax (maximum temperature), TR (temperature range), VPDavg (average VPD), VPDmax (maximum VPD), SH50 (soil humidity at 50-cm depth), SH100 (soil humidity at 100-cm depth), RF (rainfall), SR (solar radiation) and D-day (degree days). Environmental variables (fixed variables) and secondary metabolites (secondary variables) are in black arrows and red text, respectively. In the graphics (right part of the figure), the blue lines are simple linear models (n=9) with each black dot representing a trial and grey areas the confidence intervals at 95%. Represented linear regressions are cafestol (A), kahweol (B), C20:0 (C), C22:0 (D) in function of Tavg.

Figure 3. PCA and regression of climatic variables from 9 trials in the Northwest of Vietnam with volatiles from bean content of 3 genotypes, Catimor (C), Marsellea (M), and Starmaya (HS). EL (elevation), Tavg (average temperature), Tmin (minimum temperature), Tmax (maximum temperature), TR (temperature range), VPDavg (average VPD), VPDmax (maximum VPD), SH50 (soil humidity at 50-cm depth), SH100 (soil humidity at 100-cm depth), RF (rainfall), SR (solar radiation) and D-day (degree days). Environmental variables (fixed variables) and secondary metabolites (secondary variables) are in black arrows and red text, respectively. Compounds in blue and red are correlated with soil water and temperature, respectively. In the graphics (right part of the figure), the blue lines are simple linear models (n=9) with each black dot representing a trial and grey areas the confidence intervals at 95%. Represented linear regressions are benzaldehyde (A), benzene ethanol (B), 2,3-butanediol (C), ethanol (D), hexanoic acid (E), pentanoic acid (F), butyrolactone (I), phenylacetaldehyde (J), dodecane (K) in function of Tavg as well as 2,3-butanediol and dodecane in function SH50.

DISCUSSION

Genotype, environment, and genotype-environment interactions

G, E, and GxE have already been well documented for the growth and production of *C. arabica*¹⁹, but few articles have looked into their effect on the bean chemical composition^{47,48}. The presently observed contents of secondary metabolites are within the range of those already described in the literature for *C. arabica*^{1,4-8}. All compounds had a significant G effect, however only 5 secondary metabolites and 2 volatile compounds were found to have a G effect higher than the E effect (SM Fig., 4). Among them, 3,4-diCQA, 4,5-diCQA, FQA, and 5-pCoQA are chlorogenic acids, a group of chemicals associated with acidity and bitterness in coffee²⁻⁴. On the other hand, the 2-methoxy-3-isobutyl-pyrazine was already reported to be a volatile abundant in good quality coffee beans¹². Controlling the content of these compounds in coffee beans through breeding programs could improve beverage quality. The higher content of chlorogenic acids in Catimor observed in our study (SM Fig., 4), has already been reported for *C. arabica* genotypes introgressed with *C. canephora* genome³² and might be responsible for the lower beverage quality of the Catimor group.

The bean contents of the 19 compounds with E representing about 50% of the variance are most likely to be influenced by future environmental change. The effect of environmental variables on coffee bean physical characteristics, beverage quality^{3,16,49} and less frequently on bean chemical compounds^{15,19,20,22} have already been studied at the landscape and plot scale. Our study found an ANOVA's significant E effect for all measured volatile compounds including 13 compounds (acetic acid, benzaldehyde, dimethyl sulfide, toluene, ethanol, hexanal, hexanoic acid, pentanoic acid, toluene, 2-methyl furan, 3-methyl furan, 3-methyl butanoic acid, 2,3-butanediol) already identified in a past study where 40 out of 44 volatile compounds had a significant E effect²⁹.

In our present study, twenty-two bean chemical compounds and 5 bean physical characteristics had a high GxE effect. These variables decrease with temperature for one genotype but increase for another, therefore their variation is more difficult to manipulate through breeding programs and environmental management^{50,51}. However, such cross-over interactions open opportunities to define a unique terroir using an adapted genotype in a particular location.

Average temperature and soil humidity correlation with bean chemical compounds

Both temperature and soil water availability appeared to play a key role in fruit and seed development of several perennial species^{45,52,53}. In our study, we found that air temperature was more often correlated with coffee bean chemical compounds than soil humidity or rainfall. This may be explained by the high sensitivity of *C. arabica* plants to the air dryness as its photosynthesis nearly stops at VPD above 1.7 kPa and likely impairs fruit development especially in full-sun conditions⁵⁴⁻⁵⁷. Our results also revealed that long saturated fatty acids were positively correlated with temperature as already reported in coffee^{15,18,21} as well as for cacao⁵². This augmentation has been hypothesized to enable cell survival across a large range of temperatures. In our study, cafestol and kahweol, two diterpenes used as indicators of good beverage quality⁴, also correlated positively with temperature.

In coffee beverage, volatile compounds present in green beans have been mostly associated with defects and decreased beverage quality^{11,12}. The results presented here showed that 11 volatile compounds had a significant and positive correlation with Tavg while only 3 compounds were negatively correlated with Tavg. Therefore, we can state that an increasing average temperature is more likely to increase the bean concentration of volatile compounds linked to off-flavour defects in the beverage. We showed that butyrolactone (referred as associated with bean defects) was positively correlated with temperature¹¹. Despite its overall low impact on the bean chemical content, soil humidity also correlated positively with 2,3-butanediol and negatively with dodecane, highlighting its importance on bean volatile composition.

Figure 4. Scatterplot of the coefficients of determination (R^2) in function of time in weeks after flowering (WAF) for the linear regression model ($n=36$) of bean chemical compounds with the moving average of Tavg (A1, A2) and VPDavg (B1, B2) and the moving cumulative RF (C1, C2) calculated over 30 days. The dot size indicates the climate variable. Horizontal dashed black lines are the thresholds of significance for the determination coefficients ($R^2 = 0.104$).

The accumulation of chemical compounds and the bean filling response of *C. arabica* to temperature and soil humidity were previously reported to be specific to the genotype¹⁵. In the present study, we showed the absence of correlations between temperature and the bean contents of kahweol for C and S, hexanoic acid, pentanoic acid, phenylacetaldehyde, dodecane for M and ethanol, benzene ethanol for C, therefore suggesting a stability of these compounds in their genotype. Such a homeostasis of these genotypes for these compounds may be an advantage regarding warmer climate which should be privileged in replanting programs. Our multivariable approach provided us some hints regarding possible bean content differences between genotypes along a temperature gradient, however these effects could be clearer with a network of trials offering wider environmental variation. Although we observe differences between genotypes, the G effect has less influence than E on the bean chemical content. Therefore, the introduction of new genotypes is unlikely to significantly change bean chemical composition and quality of the coffee grown in this region. Other agronomical characteristics like yield and plant vigour must be assessed before choosing the genotypes to widely disseminate in the region.

Time-dependence during bean development of the correlation of environmental variables with bean chemical compounds

Despite the limited differences in annual average temperatures across trials, our approach using iterative moving average highlighted the periods when the environment may affect the most the bean chemical composition. The coffee fruit and its two beans start growing from pollination onset and reach their full size at the 19th week after flowering. At this stage, the bean starts to accumulate sucrose, fatty acids, and proteins until reaching its mature stage at around 28th WAF^{5,58}. The environmental conditions during these weeks of bean development can alter the final chemical composition of the bean^{18,21}. In our study, temperature appears to have a constant effect on the studied bean chemical compound (8-24 WAF). It is likely explained by the constant high average temperature controlling bean-filling rate, hormone activity, and the synthesizing of bean chemical components⁵⁹. The effect of temperature on chemical bean compounds decreased in the period with low average temperature, thus, cold conditions may decrease the accumulation rate of bean chemical compounds.

The average VPD correlated with bean chemical compounds during the bean size enlargement stage (6-12 WAF) when its value was high and during the bean filling stage (20-26 WAF). The rainfall was correlated with bean content of volatile compounds and secondary metabolites at different periods of the bean growth stage (8-12 and 14-18 WAF, respectively). The rainfall correlation with the volatile compounds resulted in coefficients with a high variation, sometimes shifting from positive to negative for a same compound, for instance for benzaldehyde, pentanoic acid, and phenylacetaldehyde. This is explained by the higher variance of the rainfall data compared to those of temperature and VPD. Like in our study, other authors have found that benzaldehyde correlated with high daily rainfall and they hypothesized that it repelled pests of the apple fruit⁶⁰.

The patterns of variation of the correlation coefficients over time were overall similar between compounds highlighting a universal effect of environmental conditions on all compounds and bean-filling processes. Small differences existed and highlighted a possible response of certain bean chemicals to environmental changes during the bean development. The narrow environmental differences across the studied trials can explain the small number of observed differences between chemical compounds and periods.

CONCLUSION

Using an environmental dataset from 9 trials, and a bean analysis of volatile compounds and secondary metabolites from three *C. arabica* genotypes, we identified the compounds more influenced by the

genetic make-up and the cultivation environment. We found that most compounds of the coffee beans with a significant environment effect were more influenced by variables related to temperature than variables related to soil water content. This study also highlighted the period when average temperature, VPD and cumulative rainfall mostly influenced the content of certain bean compounds. We observed that an increase in air temperature and dryness can change bean chemical composition but not necessarily bean physical characteristics. A 2°C increase in temperature altered bean chemical composition; however, genotype specific responses were evidenced and should be considered in future breeding programs to maintain coffee beverage quality in the midst of climate change.

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Conflict of Interest Statement

The authors have no conflict of interest to declare that are relevant to the content of this article.

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