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Association between higher coffee quality, bioactive chemical profile and sustainable practices

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Coffee is one of the most vulnerable crops to climate change and farming practices, since its productivity is shaped by factors such as temperature, precipitation, and soil, among others. Consequently, the final product's chemistry and quality can be significantly altered. This study investigates the hypothesis that higher coffee quality is associated with production areas implementing sustainable management practices. For that, we assessed the link between agricultural practices, sensory quality and bioactive chemical profile of coffee. *Coffea arabica* beans were sourced from two contrasting cultivation areas in Brazil. The changes in the chemical composition of the beans were assessed by targeted metabolomics, while the quality of the coffee was evaluated by sensory grading. Higher quality and higher altitudes correlated with lower levels of all xanthine alkaloids, ferulic acid and *p*-coumaric acid. Higher soil organic matter was associated with lower levels of trigonelline, theophylline, caffeine and ferulic acid. Interestingly, soil organic matter and organic carbon stock correlated positively with coffee quality. Therefore, this study demonstrates that promoting coffee production through sustainable practices contributes not only to the mitigation of effects of greenhouse gas emissions but also to the production of higher-quality coffees with increased added value.

KEYWORDS

specialty coffees, climate change, sustainability, sensory quality, secondary metabolites

1 Introduction

Brazil stands as the world's leading coffee producer and exporter, accounting for over one-third of the total global production (CONAB, 2024). With extensive cultivation areas located in southern Brazil, the state of Minas Gerais is responsible for about two-thirds of the Brazilian productivity (Tieghi et al., 2024). The southern and southwestern Brazilian regions offer coffee plantations optimal growing conditions. Indeed, successful *C. arabica* cultivation in tropical regions is influenced by a combination of environmental and crop management factors. Optimal cultivation occurs under mean annual temperatures of 14–26°C, annual precipitation ranging from 1,000 to 2,700 mm, and a distinct dry season of 1–3 months. These conditions are typically associated with altitudinal ranges of approximately 400–1,200 m above sea level in tropical regions, or 1,000–2,100 m above sea level in equatorial regions (Ahmed et al., 2021). However, those optimal conditions are being increasingly threatened by climate change, which directly affects flowering, fruit ripening, and pest incidence, impacting quality, productivity and price (Ahmed et al., 2021; Faraz et al., 2023).

Besides the natural environmental conditions, coffee's physiological growth stages are highly dependent on the nutrient availability, being nitrogen (N), phosphorus (P), and potassium (K), the primary macronutrients influencing yield and bean quality. Nitrogen, with optimal range levels varying between 51 mg/kg and 87 mg/kg is especially important for the vegetative growth; Appropriate values of potassium (ranging from 78 and 156 mg/kg) contribute to enhanced bean quality and prevents plant defoliation; Soil phosphorus, with suitable values between 10 and 20 mg/kg is essential to for enhances leaf gas exchange, photosynthesis, and overall growth of young arabica coffee plants, even under water deficit conditions (Rakocevic et al., 2022; Chilito et al., 2025).

The quality of the final product is dependent on the chemical composition of the green beans, rich in bioactive compounds such as phenolic compounds, alkaloids and diterpenes, as well as primary metabolites such as sugars, lipids and amino acids. After roasting, those compounds develop the characteristic flavor, aroma and other sensory attributes, which will give coffee the many different classifications and market value (Váradý et al., 2022).

It is well known that the relative concentration of such compounds is dependent on the combination between the genetic background, the geographical origin and environmental growing conditions (Tieghi et al., 2024). However, up to date, no study has evaluated the influence of implemented sustainable agronomic practices with the quality of the final product in terms of chemical profile of the green beans and the corresponding sensory score provided by the roasted beans. Therefore, this study examines the hypothesis that superior coffee quality is associated with production areas where sustainable management practices are

applied. It also provides preliminary insights into the relationship between local environmental factors, agricultural management, and coffee biochemistry.

2 Material and methods

2.1 Coffee beans sampling, processing and analysis

Eight samples of green (unroasted) coffee beans and their corresponding roasted counterparts were obtained from two distinct and contrasting coffee-producing regions in the state of Minas Gerais, Brazil. These included the farms of Conquista, located in the municipality of Alfenas/MG (ALF), and Rio Verde at the municipality of Conceição do Rio Verde/MG (CRV). At ALF, all the collected coffee varieties were Acaiá, whereas at CRV, the collected varieties comprised Bourbon, Catuaí, Gueisha, and Acaiá. At ALF, harvesting is mechanized, while CRV harvesting is manual and selective (Table 1). All samples were harvested and processed in 2023. The sensory evaluation was performed by Q-graders from Ipanema Coffees, following the Specialty Coffee Association (SCA) protocols (SCA - Specialty Coffee Association, 2008).

Intact coffee beans (green and roasted) were packaged in sealed plastic bags and stored at 10°C. From each sample, 10 g of beans were ground in a knife mill and the particle size was standardized using a 20 mesh granulometric sieve. The powdered samples were stored in 2.0 mL Eppendorf tubes at -20°C. An amount of 100 mg ($\pm$ 2 mg) of each sample was transferred to 1.0 mL Eppendorf tubes and extracted with 1 mL of 80% v/v methanol, containing 200 μ g/mL of naringenin as internal standard (IS), with the aid of an ultrasound bath. All samples were analysed by high-performance liquid chromatography (HPLC-UV-DAD, Shimadzu, Kyoto, Japan), in three technical replicates (n=3) exactly as described by Tieghi et al. (2024).

Chromatographic separations were carried out using a C18 chromatographic column (150 $\times$ 4.6 mm, 5 μ m, Phenomenex, Torrance, CA, USA), protected by a guard column of the same stationary phase. Purified water acidified with 0.2% of formic acid (v/v), pH 2.7 (solvent A), and methanol containing 10% of acetonitrile and 0.2% of formic acid (v/v) (solvent B) were used as mobile phase components. The elution gradient ranged from 10% to 25% of B, from 0 to 2 min, then from 25% to 50% of B from 2 to 16 min, and from 50% to 100% of B until 22 min, keeping at 100% of B until 28 min. Gradient return to initial condition (10% of B) was performed in 1 min and column re-equilibration was achieved with additional 7 min. The flow rate was 1.0 mL/min and the injection volume was 10 μ L. Detection of analytes was performed at a wavelength window ranging from 200 to 800 nm. Peaks were assigned by comparison with authentic standards retention time and UV spectra. For the quantitative analysis, peaks were integrated at 268 nm for trigonelline, 275 nm for theophylline, theobromine,

TABLE 1 Samples' varieties and origins, altitude, temperature, rainfall average, harvesting method, and characterization of the producing areas.

Sample	Variety	Municipality (Minas Gerais state)	Altitude (m)	Temperature °C	Rainfall (mm)	Harvesting method	Glebe (Ha)	pH	SOC (ton/Ha)	SOM (%)
1	Acaiá	Alfenas	856	22.01	1250	Mechanized	46	4.6	35	3.6
2	Acaiá	Alfenas	800	22.01	1250	Mechanized	32	4.2	22	2.8
3	Acaiá	Alfenas	893	22.01	1250	Mechanized	56	4.4	32	2.4
4	Acaiá	Alfenas	842	22.01	1250	Mechanized	20	4.8	44	2.5
5	Bourbon	Conceição do Rio Verde	1260	20.50	1453	Manual/selective	5	4.8	60	3.8
6	Catuai	Conceição do Rio Verde	1139	20.50	1453	Manual/selective	14	4.3	45	3.5
7	Gueisha	Conceição do Rio Verde	1227	20.50	1453	Manual/selective	11	4.8	75	3.8
8	Acaiá	Conceição do Rio Verde	1110	20.50	1453	Manual/selective	16	4.9	34	2.9

and caffeine, and 325 nm for chlorogenic acid, caffeic acid, ferulic acid, and *p*-coumaric acid.

2.2 Mapping and characterization of the studied areas

The maps of the producing regions were generated using ArcGIS 10.8 (ESRI Environmental Systems Research Institute, 2020). The land use and land cover (LULC) table (Supplementary Table S1, Supporting Information) was elaborated based on data from Collection 8 of the MapBiomas platform (MapBiomas Project, 2023), the Landsat-8 TM (Thematic Mapper) satellite images, and mappings elaborated by Ipanema Coffees. The Digital Elevation Model (DEM) (Figures 1A, B) was developed based on images with 30 m resolution from the Copernicus program, specifically GLO-30, from the X-band of the TanDEM-X and TerraSAR-X missions (ESA European Space Agency, 2024).

2.3 Soil organic matter and organic carbon analysis

Soil samples from each farm were collected from the coffee plots to determine the soil organic matter (SOM) content and soil organic carbon (SOC) stock. All the samples were collected in a disaggregated form, at a 0 to 20 cm depth, weighing around 600 g. SOM content was determined by Cooxupé laboratories using the dry quantification methodology in a muffle furnace by incineration (Sousa et al., 2018). The SOC content was estimated assuming that 58% of the SOM content consists of SOC (Van Bemmelen, 1890). According to the SOC content for each point sample, the SOC stock was determined, in Mg/ha, for each glebe, from 2019 to 2024, using the Veldkamp equation (Veldkamp, 1994), described by Equation below:

$$SOC_{stock} = \frac{SOC \times Sd \times t}{10}$$

In which: SOC_{stock} = total stock of organic C at a given depth, in this case, 0–20 cm (Mg/ha); SOC = total soil organic C content at the depth sampled (g/dm³); Sd = soil density (kg/dm³) and t = thickness of the layer considered (cm).

2.4 Statistical analysis

Comparisons between means, normality and correlation analyses were performed using Prism software (version 8.0.1, GraphPad software®, La Jolla, CA, USA). Statistical differences were considered significant if p-value < 0.05. Numerical variables were subjected to four normality tests: Anderson-Darling, D'Agostino & Pearson; Shapiro-Wilk; and Kolmogorov-Smirnov. The Mann-Whitney test was used to compare the averages between ALF and CRV samples. The heatmap was based on a correlation matrix comparing the 8 quantified compounds with geographic variables (altitude, SOM, SOC, soil pH) and sensory score. Pearson and Spearman correlation coefficients were evaluated for variables with normal and non-normal distribution, respectively. The red-blue scale was added using Microsoft® Excel® for Microsoft 365 MSO (v.2305 Build 16.0.16501.20074) software. For the multivariate data analysis, the data obtained for the green coffee beans were normalized by the IS, auto scaled and subjected to principal component analysis (PCA) using MetaboAnalyst 6.0 (Montreal, QC, Canada) (<https://www.metaboanalyst.ca/>).

3 Results

3.1 Description and characterization of the producing regions

The present study included coffee beans and metadata from two main geographical regions of Minas Gerais (Supplementary Figures

S1A, B, Supporting Information). Both areas are classified under a humid subtropical climate (Cwb) (Alvares et al., 2013). Over the past five years, based on meteorological and pluviometry measurements in the study area, ALF and CRV recorded an annual average temperature of 22.01°C and 20.50°C and an average yearly rainfall of 1250 mm and 1453 mm, respectively. The LULC classes are presented in Supplementary Table S1 (Supporting Information). Due to the flat topography and good spacing between the plants, mechanized harvesting is next to 100% at ALF and 69% at CRV, which enables lower operational costs. In CRV, manual or semi-manual picking is used to harvest the ripe

cherries. The general differences between the two harvesting methods are presented in Supplementary Figure S2 (Supporting Information). In ALF, the spacing between planting rows and same row plants varied from 3.5 to 4.0 m and from 0.5 to 1.0 m, respectively; in CRV, spacing between planting rows and plants within the same row varied from 2.0 to 4.0 m and from 0.5 to 2.0 m, respectively. Both coffee production areas are in a full sun model, managed with agronomic practices including fertilization, weed, pest and disease control, pruning management, irrigation and post-harvest treatments. The average altitude of CRV is significantly higher ($p = 0.029$) than that of ALF, as can be seen in Figures 1A, B,

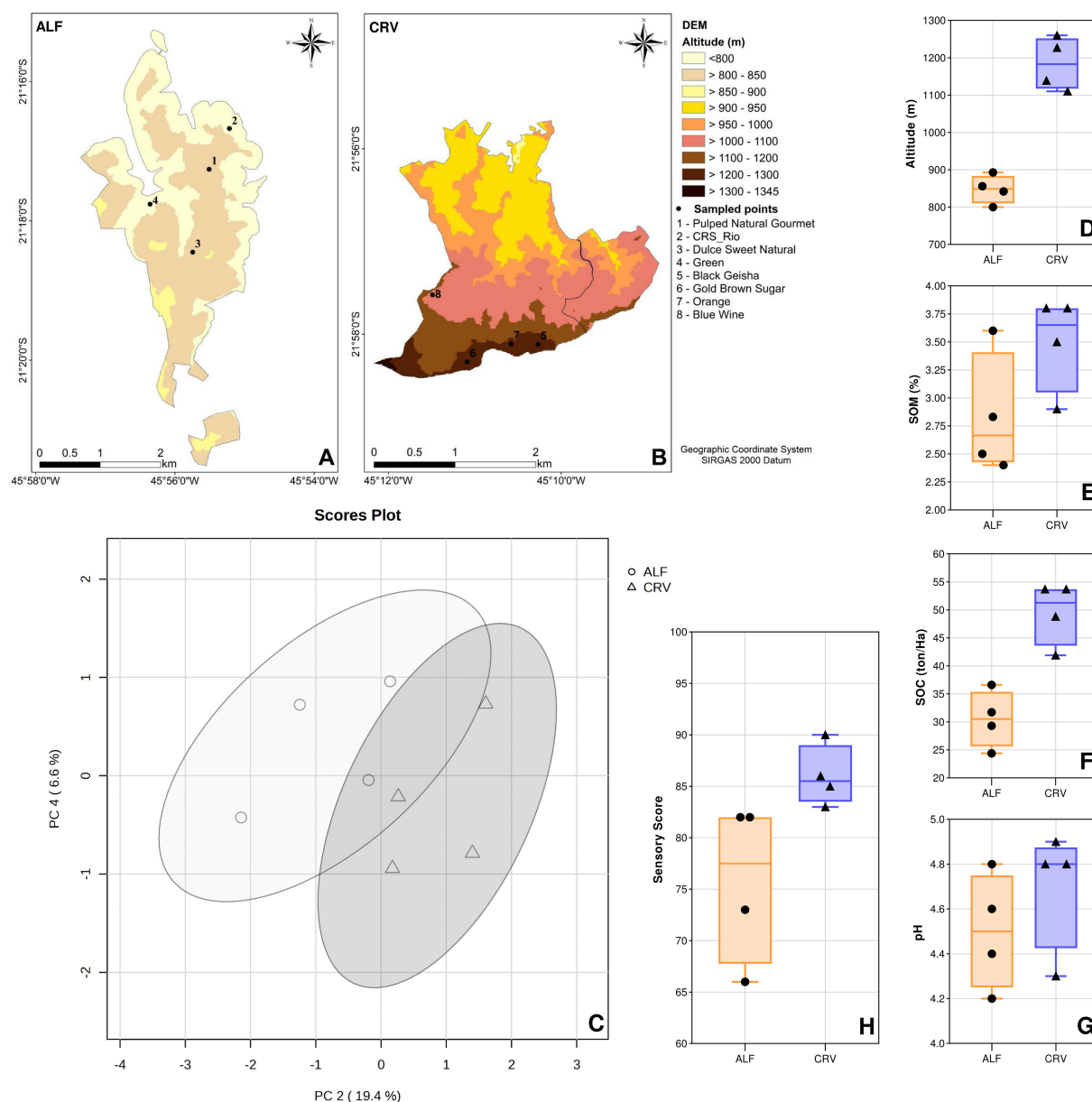


FIGURE 1

Comparison between coffee samples from two farms located in Alfenas-MG (ALF; $n = 4$) and Conceição do Rio Verde-MG (CRV; $n = 4$). (A) Altitude map of ALF and (B) CRV showing the samples' locations. (C) PCA score plot based on the samples' chemical profile; (D) Box-plots representing Mann-Whitney test comparing samples from ALF and CRV regarding altitude (p -value = 0.029); (E) soil organic matter - SOM (p -value = 0.114); (F) soil organic carbon - SOC (p -value = 0.029); (G) soil pH (p -value = 0.314) and (H) sensory score (p -value = 0.029).

D. Regarding soil, SOC was significantly higher at CRV ($p = 0.029$, Figure 1F), while SOM and pH were shown to be statistically equivalent ($p = 0.114$ and $p = 0.314$, respectively) (Figures 1E, G, respectively). Both SOC and SOM correlated positively with altitude (Figure 2B, C, respectively).

3.2 Chemical profile characterization of green and roasted beans and sensory quality

The chemical analysis of the green and roasted beans (Figure 3, Supplementary Table S2, Supporting Information) shows significant differences in the content of all compounds, except for caffeine ($n=8$). After roasting, the content of all phenolic compounds and trigonelline increase, whereas the content of theophylline and theobromine is reduced. An unsupervised multivariate data analysis (PCA) revealed subtle differences between the chemical composition of the green coffees produced in the two regions. While the first two principal components (PC1 and PC2) explained 82.6% of the data variability, the better separation between samples farms was observed when comparing

PC2 and PC4, as confirmed by PERMANOVA analysis (999 permutations; $F = 5.0636$; $r^2 = 0.45768$; $p = 0.028$). The differences in the chemical composition between the two regions were primarily captured by PC2. According to the PC2 loadings, trigonelline, ferulic acid, and *p*-coumaric acid were the most influential compounds contributing to the differentiation between the two farms. Caffeine and chlorogenic acid, which are the two major compounds found in both green and roasted beans did not influence the separation (Supplementary Table S3, Supporting Information). Coffees from CRV presented higher sensory scores than those from ALF (Figure 1H), with a statistically significant difference according to the Mann-Whitney test ($p = 0.029$).

3.3 Correlation analysis between the chemical profile, geographical origin, and sensory quality

The correlation coefficients related to the chemical profile, geographic aspects, and sensory score are shown in the heatmap of Figure 2A. Lower levels of all xanthine alkaloids, ferulic acid and *p*-coumaric acid were associated to higher quality and higher

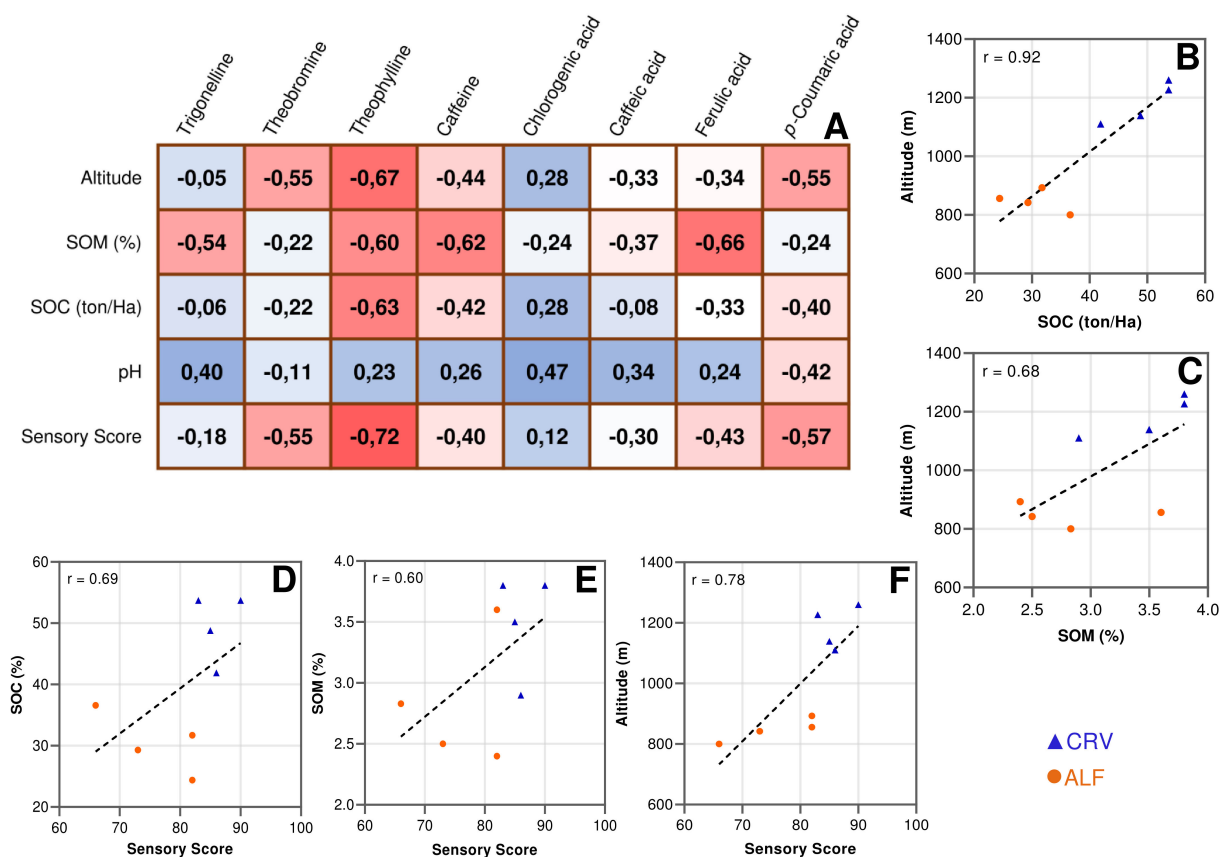


FIGURE 2

(A) Correlation analysis between chemical composition of the green coffee beans and geographical variables: Heatmap based on correlation coefficients comparing chemical profile and geographical variables; (B) Correlation analysis between altitude and soil organic carbon (SOC); (C) Correlation analysis between altitude and soil organic matter (SOM); (D) Correlation analysis between SOC and sensory score; (E) Correlation analysis between SOM and sensory score; (F) Correlation analysis between altitude and sensory score.

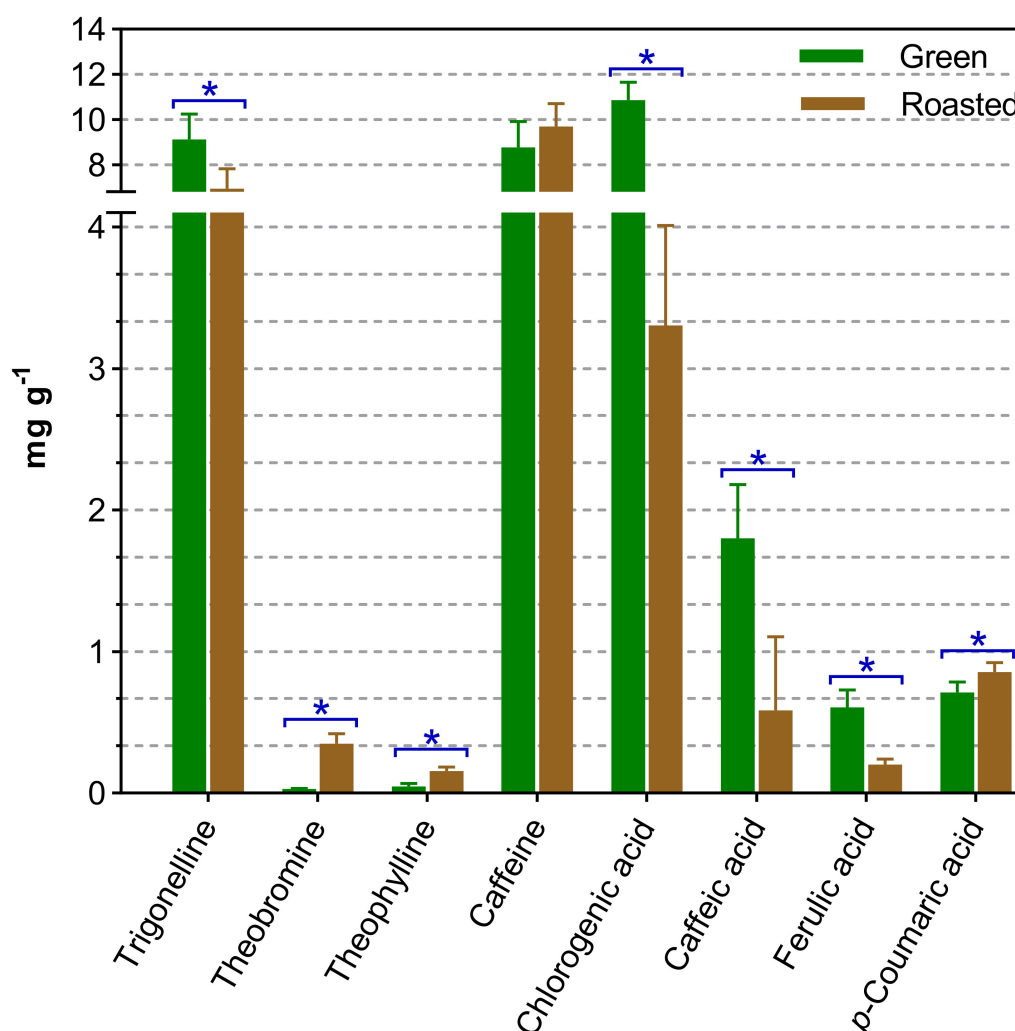


FIGURE 3

Quantitative analysis of target secondary metabolites present on green and corresponding roasted coffee beans (n=8). *Significant at $p < 0.05$.

altitudes. Coffee quality (sensory score) correlated positively with organic carbon stock, soil organic matter and altitude (Figures 2D–F, respectively). Higher soil organic matter was associated with lower levels of trigonelline, theophylline, caffeine and ferulic acid. However, only theophylline showed stronger negative correlation with soil carbon storage. Chlorogenic acid derivatives were positively correlated with higher soil pH.

4 Discussion

The non-supervised multivariate data analysis (PCA) indicated the feasibility of distinguishing coffees originating from two distinct producing regions based on the concentrations of eight bioactive compounds (four alkaloids and four phenolic compounds) (Figure 1C). It is worth noting that the chemical information preserved within the green beans was utilized for this purpose. Roasting transforms the chemical composition of green beans into volatile and non-volatile compounds responsible for the aroma and

flavor of a cup of coffee. The main chemical reactions involve the decomposition of sugars, oxidation of lipids, pyrolysis, and the Maillard reaction (Angeloni et al., 2021; Moon et al., 2025). Chlorogenic acid was the most abundant compound quantified in the present study and underwent substantial degradation during roasting (Liao et al., 2022). Its degradation is expected as it is an unstable ester of caffeic acid and quinic acid, easily converted into these two compounds in the roasting process. Subsequent reactions give rise to a variety of volatile compounds, such as phenol, benzoic acid, catechols and their derivatives, as well as non-volatile compounds, including quinic acid epimers and lactone derivatives of chlorogenic acids (Viencez et al., 2023). These compounds collectively contribute to the sensory characteristics of the coffee (Hu et al., 2020). Additionally, a decrease in caffeic acid levels was observed, consistent with previous studies on roasting processes (Alcantara et al., 2025; Rzycka-Szczupak et al., 2025). Trigonelline, the second most abundant compound quantified in this study, also underwent decomposition during roasting. Its degradation generates flavor and aroma desirable products, including furans,

pyrazines, alkyl-pyridines, and pyrroles (Toci et al., 2020; Wu et al., 2022). Following the abundance sequence, the caffeine content did not change significantly during roasting. This observation is expected given its well-established stability in the literature (Tarigan et al., 2022). The other evaluated metabolites underwent statistically significant but biologically subtle alterations.

Notably, the chemical constituents measured in the green bean exhibited correlations with altitude, SOM, SOC, and the overall quality of the brewed beverage (Figure 2A). These findings offer a chemical rationale for the different cultivation and environmental conditions shown by the two contrasting locations, and their influence on the sensory attributes of the final beverage (coffee after roasting and extraction). Trigonelline, ferulic acid, and *p*-coumaric acid were the principal chemical constituents responsible for distinguishing the geographical origin of the coffee beans. From those, *p*-coumaric acid, in addition to all xanthine alkaloids (theobromine, theophylline and caffeine) showed stronger negative correlation with altitude (Figure 2A). Interestingly, coffee exhibiting reduced concentrations of these compounds were also associated with higher sensory scores. Higher soil organic matter was associated with lower levels of trigonelline, theophylline, caffeine and ferulic acid. Our observations are consistent with the lower content of caffeine and trigonelline in coffees grown in richest organic matter soil observed by Gebrekidan et al. (2019). Unprecedentedly, we also report a negative correlation between theophylline and ferulic acid with organic matter in soil. Interestingly, soil organic matter and organic carbon stock correlated positively with coffee quality. Those findings revealed that high-quality coffee beans presented reduced concentrations of xanthine derivatives, in addition to *p*-coumaric acid. Coffee beans possessing relatively lower amount of those compounds in the green beans were predominantly sourced from elevated regions with soils enriched in organic matter, reinforcing the observation that coffees cultivated at CRV, a farm characterized by higher altitude and higher SOC content, consistently achieved superior sensory score.

From the agricultural practices' perspective, although SOM content is statistically similar between the two farms, SOC levels are significantly higher in CRV. It is noteworthy to mention that the higher average soil organic carbon (SOC) stock observed in the CRV region (Figures 1F, 2B) can be partially attributed to its elevated altitude. Cooler climates at higher altitudes tend to suppress microbial activity, thereby slowing the decomposition rate of soil organic matter (SOM) and enhancing SOC sequestration (Li et al., 2022; Pellikka et al., 2023). Both SOM and SOC play a critical role in improving crop yields and creating favorable soil conditions for coffee cultivation (Sousa et al., 2018; Tasew et al., 2021; Freitas et al., 2024). Besides, the adoption sustainable agricultural management practices at CRV also promotes SOC accumulation through several measures: (i) maintaining vegetation cover interspersed within cultivation areas; (ii) reducing the spacing between rows to increase plant density; (iii) practicing manual harvesting in steep areas to minimize soil compaction; (iv) enhancing the incorporation of plant residues into the soil; and (v) maintaining higher biomass

in the cultivated plants. These practices not only increase SOC levels but also improve soil nitrogen (N) retention, thereby reducing the dependence on synthetic fertilizers (Tasew et al., 2021; Yin et al., 2022).

In addition, other agronomic practices employed in CRV may contribute to improved crop quality. These include (i) selective harvesting at optimal ripening stages, (ii) close monitoring of climatic conditions, (iii) annual soil and foliar analyses, (iv) efficient fertilizer application, and (v) proper post-harvest storage of beans (Worku et al., 2018; Alliance for Coffee Excellence, 2023). Collectively, these measures help reduce pest incidence and promote the development of denser, higher-quality beans (Cheng et al., 2016). They also contribute to prolonged fruit ripening and improved soil drainage, resulting in beans enriched with complex sugars, acids, and amino acids that enhance the sensory characteristics of the final beverage (Matiello et al., 2005; Vaast et al., 2006).

Those observations are corroborated by a previous study from Silveira et al. (2016), which concluded that altitude, associated with good agricultural management practices, were the major factors influencing coffee quality in Matas de Minas (Silveira et al., 2016). However, it is important to mention that altitude, temperature and rainfall may not directly impact beverage quality; instead, they can create the best environmental conditions for growing coffee (Gumecindo-Alejo et al., 2021).

It is important to highlight that both regions included in the present study favours the cultivation of *C. arabica*. However, the suitability of a region for coffee cultivation depends on several factors. Even within the same favourable areas, significant variations arise from microclimates, soil characteristics, and management practices. In our study, the region of Alfenas has lower altitudes and higher temperatures, which accelerates the maturation cycle, and potentially reducing the accumulation of sugars and aromatic compounds (Ramalho et al., 2018). In Conceição do Rio Verde, higher altitudes and cooler climate prolong maturation, allowing for a greater development of flavour complexity, vibrant acidity, and a richer aromatic profile, which are commonly associated to specialty coffees profiles. It is worth noting that the sensory analysis of roasted beans from each farm reflected the chemistry of the original green beans, revealing clear differences in cup quality and in the corresponding aromas and flavors – samples from CRV showing higher sensory score in comparison to samples from ALF. Interestingly, the samples from ALF showed higher variation among the sensory scores in comparison with the samples from CRV (Figure 1H). That result may suggest that the higher variation in the sensory score of samples from ALF might be due to the general management practices employed on that farm. Finally, attention should also be drawn to the fact that coffee is a highly demanding crop, and nutrients availability can still alter its physiological development. Hence, the application of appropriate fertilization regimes is important to fulfil the nutritional demands of coffee throughout its vegetative and reproductive stages, supporting optimal photosynthetic performance, and contributing to higher yields and superior bean quality (Li et al., 2023).

5 Conclusion

The present study identifies a relationship between sustainable management practices, coffee bioactive chemical profile and quality. Although further research is currently ongoing to deepen the understanding, the results suggest that the chemical information preserved within the green beans can be associated with altitude, SOM, SOC, and the overall quality of the final beverage. Notably, while trigonelline, ferulic acid, and *p*-coumaric acid were the principal chemical constituents responsible for distinguishing the geographical origin of the coffee beans, lower levels of all xanthine alkaloids in addition to ferulic and *p*-coumaric acid were associated to higher quality and higher altitudes, providing a chemical rationale for the observed variations in coffee quality across different farms and production regions.

A limitation of this study is the relatively small sample size, which may affect statistical power and is characteristic of pilot studies. However, a key strength of our research lies in its evaluation of the hypothesis that sustainable management practices significantly influence coffee cup quality. Furthermore, this study established a methodological framework for investigating this relationship. Future research expanding the analysis of the chemical composition through untargeted metabolomics, combined with a broader range of management practices, environmental factors, and beverage quality metrics, will contribute to a more comprehensive understanding of the chemical mechanisms underpinning coffee quality and its association with sustainable agricultural practices.

Data availability statement

The original contributions presented in the study are included in the article/**Supplementary Material**. Further inquiries can be directed to the corresponding author.

Author contributions

GV: Data curation, Methodology, Visualization, Writing – original draft, Writing – review & editing. DS: Data curation, Conceptualization, Software, Writing – original draft, Writing – review & editing. LP: Formal analysis, Methodology, Writing – original draft, Writing – review & editing. HT: Investigation, Visualization, Writing – original draft, Writing – review & editing. VS: Formal analysis, Methodology, Writing – original draft, Writing – review & editing. JA: Supervision, Investigation, Writing – original draft, Writing – review & editing. DD: Supervision, Conceptualization, Resources, Writing – review & editing. MS: Supervision, Conceptualization, Resources, Writing – review & editing. DC-P: Supervision, Conceptualization, Project administration, Resources, Funding acquisition, Writing – review & editing. RM: Supervision, Project administration, Writing – original draft, Writing – review & editing. PB: Supervision,

Conceptualization, Project administration, Funding acquisition, Writing – original draft, Writing – review & editing.

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Conflict of interest

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Supplementary material

The Supplementary Material for this article can be found online at: <https://www.frontiersin.org/articles/10.3389/fagro.2025.1645329/full#supplementary-material>

References

- Ahmed, S., Brinkley, S., Smith, E., Sela, A., Theisen, M., Thibodeau, C., et al. (2021). Climate Change and Coffee Quality: Systematic Review on the Effects of Environmental and Management Variation on Secondary Metabolites and Sensory Attributes of *Coffea arabica* and *Coffea canephora*. *Front. Plant Sci.* 12, 708013. doi: 10.3389/fpls.2021.708013
- Alcantara, G. M. R. N., Martins, L. C., Gomes, W. P. C., Dresch, D., Rocha, F. R. P., and Melchert, W. R. (2025). Effect of roasting on chemical composition of coffee. *Food Chem.* 477, 143169. doi: 10.1016/j.foodchem.2025.143169
- Alliance for Coffee Excellence (2023). Brazil 2023. Available online at: <https://allianceforcoffeexcellence.org/Brazil-2023/> (Accessed May 29, 2024).
- Alvares, C. A., Stape, J. L., Sentelhas, P. C., De Moraes Gonçalves, J. L., and Sparovek, G. (2013). Köppen's climate classification map for Brazil. *Meteorologische. Z.* 22, 711–728. doi: 10.1127/0941-2948/2013/0507
- Angeloni, S., Mustafa, A. M., Abouelenein, D., Alessandrini, L., Acquaticci, L., Nzekoue, F. K., et al. (2021). Characterization of the aroma profile and main key odorants of espresso coffee. *Molecules* 26, 3856. doi: 10.3390/molecules26133856
- Cheng, B., Furtado, A., Smyth, H. E., and Henry, R. J. (2016). Influence of genotype and environment on coffee quality. *Trends Food Sci. Technol.* 57, 20–30. doi: 10.1016/j.tifs.2016.09.003
- Chiloto, E. D. L., Olaya, J. F. C., Corrales, J. C., and Figuero, C. (2025). Sustainability-driven fertilizer recommender system for coffee crops using case-based reasoning approach. *Front. Sustain. Food Syst.* 8, 1445795. doi: 10.3389/fsufs.2024.1445795
- CONAB (2024). Boletim da safra de grãos. 12º levantamento. Available online at: <https://www.conab.gov.br/info-agro/safas/graos/boletim-da-safra-de-graos> (Accessed July 17, 2024).
- ESA European Space Agency (2024). Copernicus Data. Available online at: https://www.esa.int/Applications/Observing_the_Earth/Copernicus (Accessed January 24, 2024).
- ESRI Environmental Systems Research Institute (2020). ARCGIS Professional GIS for the desktop v.10.8. (Version 10.8) [software]. (Redlands, California, USA). Available online at: <https://www.arcgis.com/index.html> (Accessed March 24, 2024).
- Faraz, M., Mereu, V., Spano, D., Trabucco, A., Marras, S., and El Chami, D. (2023). A systematic review of analytical and modelling tools to assess climate change impacts and adaptation on coffee agrosystems. *Sustain* 15, 14582. doi: 10.3390/su151914582
- Freitas, V. V., Borges, L. L. R., Vidigal, M. C. T. R., dos Santos, M. H., and Stringheta, P. C. (2024). Coffee: A comprehensive overview of origin, market, and the quality process. *Trends Food Sci. Technol.* 146, 104411. doi: 10.1016/j.tifs.2024.104411
- Gebrekidan, M., Redi-Abshiro, M., Chandravanshi, B., Ele, E., Mohammed, A., and Mammo, M. (2019). Influence of altitudes of coffee plants on the alkaloids contents of green coffee beans. *Chem. Int.* 5, 247–257. doi: 10.5281/zenodo.2604404
- Gumecindo-Alejo, A. L., Sánchez-Landero, L. A., Ortiz-Ceballos, G. C., Cerdán-Cabrera, C. R., and Alvarado-Castillo, G. (2021). Factors related to coffee quality, based on the “cup of excellence” contest in Mexico. *Coffee. Sci.* 16, e161887. doi: 10.25186/v.16i.1887
- Hu, G., Peng, X., Gao, Y., Huang, Y., Li, X., Su, H., et al. (2020). Effect of roasting degree of coffee beans on sensory evaluation: Research from the effect of major chemical ingredients. *Food Chem.* 331, 127329. doi: 10.1016/j.foodchem.2020.127329
- Li, R., Cheng, J., Liu, X., Wang, Z., Li, H., Guo, J., et al. (2023). Optimizing drip fertigation at different periods to improve yield, volatile compounds and cup quality of Arabica coffee. *Front. Plant Sci.* 14. doi: 10.3389/fpls.2023.1148616
- Li, C., Xiao, C., Li, M., Xu, L., and He, N. (2022). A global synthesis of patterns in soil organic matter and temperature sensitivity along the altitudinal gradient. *Front. Environ. Sci.* 10. doi: 10.3389/fenvs.2022.959292
- Liao, Y. C., Kim, T., Silva, J. L., Hu, W.-Y., and Chen, B.-Y. (2022). Effects of roasting degrees on phenolic compounds and antioxidant activity in coffee beans from different geographic origins. *LWT-Food. Sci. Technol.* 168, 113965. doi: 10.1016/j.lwt.2022.113965
- MapBiomass Project (2023). Coleção 8 da Série Anual de Mapas de Cobertura e Uso da Terra do Brasil. Available online at: <https://brasil.mapbiomas.org/> (Accessed July 19, 2024).
- Matiello, J. B., Santinato, R., Garcia, A. W. R., Almeida, S. R., and Fernandes, D. R. (2005). *Cultura de café no Brasil: novo manual de recomendações. 1st ed.* (Rio de Janeiro/Varginha: MAPA/PROCAFÉ).
- Moon, S. A., Wongsakul, S., Kitazawa, H., and Saengrayap, R. (2025). Impact of roasting and storage conditions on the shelf stability of thai arabica coffee. *J. Agric. Food Res.* 22, 102060. doi: 10.1016/j.jafr.2025.102060
- Pellikka, P., Luotamo, M., Sädekoski, N., Hietanen, J., Vuorinen, I., Räsänen, M., et al. (2023). Tropical altitudinal gradient soil organic carbon and nitrogen estimation using Specim IQ portable imaging spectrometer. *Sci. Total. Environ.* 883, 163677. doi: 10.1016/j.scitotenv.2023.163677
- Rakocevic, M., Marchiori, P. E. R., Zambrosi, F. C. B., MaChado, E. C., Maia, A., de, H. N., et al. (2022). High phosphorus supply enhances leaf gas exchange and growth of young Arabica coffee plants under water deficit. *Exp. Agric.* 58, e30. doi: 10.1017/S0014479722000266
- Ramalho, J. C., Pais, I. P., Leitão, A. E., Guerra, M., Reboredo, F. H., Mâguas, C. M., et al. (2018). Can elevated air [CO₂] conditions mitigate the predicted warming impact on the quality of coffee bean? *Front. Plant Sci.* 9, 287. doi: 10.3389/fpls.2018.00287
- Rzyska-Szczupak, K., Przybylska-Balcerek, A., Buško, M., Szwajkowska-Michalek, L., Szablewski, T., and Stuper-Szablewska, K. (2025). Roasting temperature as a factor modifying the caffeine and phenolic content of Ethiopian coffee. *Processes* 13, 2037. doi: 10.3390/pr13072037
- SCA - Specialty Coffee Association (2008). Protocolo para Análise Sensorial de Café. Available online at: https://coffeetraveler.net/wp-content/files/901-SCAA_CuppingProtocols_TSC_DocV_RevDec08_Portuguese.pdf (Accessed December 16, 2023).
- Silveira, A. d. S., Pinheiro, A. C. T., Ferreira, W. P. M., da Silva, L. J., dos Santos Rufino, J. L., and Sakiyama, N. S. (2016). Sensory analysis of specialty coffee from different environmental conditions in the region of matas de minas, minas gerais, Brazil. *Rev. Ceres.* 63, 436–443. doi: 10.1590/0034-737X201663040002
- Sousa, J. S., Neves, J. C. L., Martinez, H. E. P., and Alvarez, V. H. V. (2018). Relationship between coffee leaf analysis and soil chemical analysis. *Rev. Bras. Cienc. Solo.* 42, e0170109. doi: 10.1590/18069657rbcs20170109
- Tarigan, E. B., Wardiana, E., Hilmi, Y. S., and Komarudin, N. A. (2022). "The changes in chemical properties of coffee during roasting: A review." in *IOP conference series: Earth and environmental science*; 2021 Sep 2-3; Borgor, Indonesia. (Indonesia. Bristol: IOP Publishing), vol. 974, 012115. doi: 10.1088/1755-1315/974/1/012115
- Tassew, A. A., Yadessa, G. B., Bote, A. D., and Obso, T. K. (2021). Influence of location, elevation gradients, processing methods, and soil quality on the physical and cup quality of coffee in the Kafa Biosphere Reserve of SW Ethiopia. *Heliyon* 7, e07790. doi: 10.1016/j.heliyon.2021.e07790
- Tieghi, H., Pereira, L., de, A., Viana, G. S., Katchborian-Neto, A., Santana, D. B., et al. (2024). Effects of geographical origin and post-harvesting processing on the bioactive compounds and sensory quality of Brazilian specialty coffee beans. *Food Res. Int.* 186, 114346. doi: 10.1016/j.foodres.2024.114346
- Toci, A. T., Azevedo, D. A., and Farah, A. (2020). Effect of roasting speed on the volatile composition of coffees with different cup quality. *Food Res. Int.* 137, 109546. doi: 10.1016/j.foodres.2020.109546
- Vaast, P., Bertrand, B., Perriot, J. J., Guyot, B., and Génard, M. (2006). Fruit thinning and shade improve bean characteristics and beverage quality of coffee (*Coffea arabica* L.) under optimal conditions. *J. Sci. Food Agric.* 86, 197–204. doi: 10.1002/jsfa.2338
- Van Bemmelen, J. M. (1890). Ueber die Bestimmung des Wassers, des Humus, des Schwefels, der in den kolloidalen Silikaten gebundenen Kieselsäure, und des Mangans, im Ackerboden. *Landwirtsch. Versuchsstat.* 37, 279–290. Available online at: <https://edepot.wur.nl/211282> (Accessed May 15, 2024).
- Várady, M., Tauchen, J., Fraňková, A., Klouček, P., and Popelka, P. (2022). Effect of method of processing specialty coffee beans (natural, washed, honey, fermentation, maceration) on bioactive and volatile compounds. *Lebensm. Wiss. Technol.* 172, 114245. doi: 10.1016/j.lwt.2022.114245
- Veldkamp, E. (1994). Organic Carbon Turnover in Three Tropical Soils under Pasture after Deforestation. *Soil Sci. Soc. Am. J.* 58, 175–180. doi: 10.2136/sssaj1994.03615995005800010025x
- Viencz, T., Acre, L. B., Rocha, R. B., Alves, E. A., Ramalho, A. R., and de Toledo Benassi, M. (2023). Caffeine, trigonelline, chlorogenic acids, melanoidins, and terpenes contents of *Coffea canephora* coffees produced in the Amazon. *J. Food Compos. Anal.* 117, 105140. doi: 10.1016/j.jfca.2023.105140
- Worku, M., de Meulenaer, B., Duchateau, L., and Boeckx, P. (2018). Effect of altitude on biochemical composition and quality of green arabica coffee beans can be affected by shade and postharvest processing method. *Food Res. Int.* 105, 278–285. doi: 10.1016/j.foodres.2017.11.016
- Wu, H., Lu, P., Liu, Z., Sharifi-Rad, J., and Suleria, H. A. (2022). Impact of roasting on the phenolic and volatile compounds in coffee beans. *Food Sci. Nutr.* 10, 2408–2425. doi: 10.1002/fsn3.2849
- Yin, S., Wang, C., and Zhou, Z. (2022). Globally altitudinal trends in soil carbon and nitrogen storages. *Catena* 210, 105870. doi: 10.1016/j.catena.2021.105870