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Geographical Variation in Volatile Compound Profiles of Pulu Mandoti Aromatic Glutinous Rice (Oryza sativa L.) Cultivated at Four Highland Sites in Enrekang, Indonesia, Revealed by HS-SPME–GC/MS

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Research Article

Keywords: Terroir, Chemometrics, Soil Geochemistry, 2-Acetyl-1-pyrroline, Landrace

Posted Date: November 26th, 2026

DOI: https://doi.org/10.21203/rs.3.rs-11336685/v1

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Additional Declarations: No competing interests reported.

Geographical Variation in Volatile Compound Profiles of Pulu Mandoti Aromatic Glutinous Rice (*Oryza sativa* L.) Cultivated at Four Highland Sites in Enrekang, Indonesia, Revealed by HS-SPME–GC/MS

Abstract

Pulu Mandoti is an endemic aromatic glutinous rice from Enrekang Regency, South Sulawesi, Indonesia, with high cultural and economic value. Local communities believe that the distinctive aroma of this variety diminishes when cultivated outside its region of origin; however, scientific evidence supporting this claim remains limited. This study aimed to characterize the volatile compound profiles of *Pulu Mandoti* rice cultivated at four highland locations (750–1,054 m above sea level) in Baraka District, Enrekang Regency, and to explore their associations with soil geochemical characteristics. We analyzed volatile compounds using headspace solid-phase microextraction gas chromatography mass spectrometry (HS-SPME–GC/MS) and analyzed 14 soil geochemical parameters in parallel. We tentatively identified compounds by matching their mass spectra against the NIST14 library (Metabolomics Standards Initiative Level 2), then analyzed the data using principal component analysis (PCA), partial least squares discriminant analysis (PLS-DA), hierarchical cluster analysis, and Spearman correlation analysis. We identified 172 volatile compounds, of which 23 constituted the core volatilome, and 105 (61%) were location-specific. PCA of the core volatilome explained 82.46% of the total variance and descriptively indicated differences in volatile composition patterns among locations. In contrast, PLS-DA identified (R)-3-cyclohexen-1-ol, 4-methyl-1-(1-methylethyl), nonanal, an octahydronaphthalene derivative, 2-octenal, 2-butyl, and butyl butanoate as candidate marker compounds. Although 2-acetyl-1-pyrroline (2-AP) was not detected, distribution of compounds analogous or structurally related to 2-AP varied across locations. Correlation analysis suggested associations between soil geochemistry and volatile compound profiles, although these relationships remained descriptive. These findings provide a scientific basis for developing geographical authentication and traceability systems, as well as conservation strategies, for *Pulu Mandoti* rice.

Keywords: Terroir, Chemometrics, Soil Geochemistry, 2-Acetyl-1-pyrroline, Landrace.

1 Introduction

Aroma is one of the most important quality attributes of rice, strongly influencing consumer preference, market competitiveness, and economic value, particularly for aromatic rice. Rice aroma results from a complex mixture of volatile compounds, including aldehydes, alcohols, ketones, esters, hydrocarbons, terpenoids, and heterocyclic compounds. Among these compounds, 2-acetyl-1-pyrroline (2-AP) is recognized as a major contributor to the characteristic aroma of aromatic rice, producing a distinctive pandan-like or popcorn-like scent that characterizes many premium cultivars. (Hu et al., 2020; Kasote et al., 2021). Although genetic factors strongly influence the presence of 2-AP, environmental conditions during plant growth also affect volatile compound accumulation in rice, including soil characteristics, cultivation location, climatic conditions, and agronomic practices. (Hu et al., 2020; Du et al., 2018). Therefore, the volatile profile of rice results from a complex interaction between genetic and environmental factors.

In recent years, the concept of terroir, referring to the influence of environmental characteristics on the chemical and sensory properties of agricultural products, has increasingly been applied in research on aromatic rice. Variation in elevation, soil physicochemical properties, microclimate, and agroecological conditions can influence plant secondary metabolic pathways, resulting in differences in volatile compound composition among cultivation regions. (Zhou et al., 2022; Asimi et al., 2022). In line with these developments, volatile metabolomics based on headspace solid-phase microextraction gas chromatography mass spectrometry (HS-SPME–GC/MS), combined with chemometric approaches such as Principal Component Analysis (PCA) and Partial Least Squares Discriminant Analysis (PLS-DA), has become widely used for geographical authentication, origin discrimination, and quality assessment of aromatic rice. These approaches have successfully differentiated the geographical origins of rice from China, Vietnam, India, and Japan based on their volatile compound fingerprint profiles (Ch et al., 2020; Asimi et al., 2022; Hu et al., 2023; Tanaka et al., 2025).

One Indonesian local genetic resource with high economic and cultural value is Pulu Mandoti, an endemic aromatic glutinous rice traditionally cultivated in Salukanan Village and surrounding areas of Baraka District, Enrekang Regency, South Sulawesi, Indonesia. In addition to being recognized for its distinctive aroma, Pulu Mandoti is strongly associated with local cultural traditions and has therefore become an important commodity in social, cultural, and economic contexts (Kusbiantoro and Handoko, 2024). Previous studies have investigated various aspects

of Pulu Mandoti, including its genetic, microbiological, and socioeconomic characteristics (Riadi et al., 2022; Hafsan et al., 2023). However, information on its volatile compound composition, particularly how variation in cultivation location influences its volatile profile, remains very limited. Most studies on aromatic rice volatiles have focused on comparisons among well-known varieties, such as Basmati and Jasmine, as well as traditional cultivars from India and China (Ashokkumar et al., 2020; Kasote et al., 2021; Zhou et al., 2022). Whereas studies evaluating intra-varietal variation within a single endemic cultivar in response to differences in growing environments remain scarce.

Local communities, meanwhile, believe that the distinctive aroma of Pulu Mandoti diminishes when the variety is cultivated outside its traditional growing area. This belief has been passed down through generations and has become a foundation for conserving traditional cultivation areas. Nevertheless, to date, no scientific evidence has systematically evaluated whether variation in cultivation location actually results in changes in volatile compound composition that could explain this phenomenon. Furthermore, no study has integrated volatile profile characterization with soil geochemical characteristics to investigate potential associations between edaphic conditions and aroma formation in Pulu Mandoti.

Accordingly, two major knowledge gaps remain. First, information on variation in the volatile compound profiles of Pulu Mandoti across different cultivation locations within its native production area remains limited. Second, the relationship between soil geochemical variation and volatile compound formation in this endemic cultivar has not yet been comprehensively evaluated using metabolomic and chemometric approaches. Unlike previous studies, which have generally compared different cultivars or geographically distinct regions, the present study focuses on intra-varietal variation within a single endemic cultivar by integrating HS-SPME–GC/MS analysis, chemometric analysis, and soil geochemical characterization. This integrated approach is expected to provide deeper insights into how the growing environment influences the formation of Pulu Mandoti's volatile fingerprint and to support the development of volatile compound-based geographical authentication.

We hypothesized that differences in soil geochemical characteristics and agroecological conditions among the four cultivation locations would produce distinct volatile compound profiles, even though all samples originated from the same cultivar. Therefore, this study aimed to (1) identify and characterize the volatile compound profile of Pulu Mandoti aromatic glutinous rice using HS-SPME–GC/MS, (2) evaluate geographical variation in volatile profiles across four cultivation locations, (3) identify discriminant markers with potential applications in geographical authentication through chemometric analysis, and (4) explore the relationships between soil geochemical characteristics and volatile compound formation. The findings are expected to provide the first volatile fingerprint of Pulu Mandoti and establish a scientific basis for geographical authentication, the development of a Geographical Indication (GI), germplasm conservation, and value addition for this endemic Indonesian aromatic rice.

2 Materials and methods

2.1 Study sites and sample collection

This study was conducted at four Pulu Mandoti cultivation sites in Baraka District, Enrekang Regency, South Sulawesi, Indonesia, representing an altitudinal gradient within the variety's region of origin. The study sites comprised (Fig. 1): (1) Salongge Hamlet, Kendenan Village (3.39531° S, 119.92302° E; 1,054 m a.s.l.); (2) Awo Hamlet, Kendenan Village (3.39160° S, 119.91085° E; 965 m a.s.l.); (3) Gandeng Hamlet, Salukanan Village (3.38927° S, 119.90138° E; 867 m a.s.l.); and (4) Kaduasik Hamlet, Salukanan Village (3.38617° S, 119.89455° E; 750 m a.s.l.).

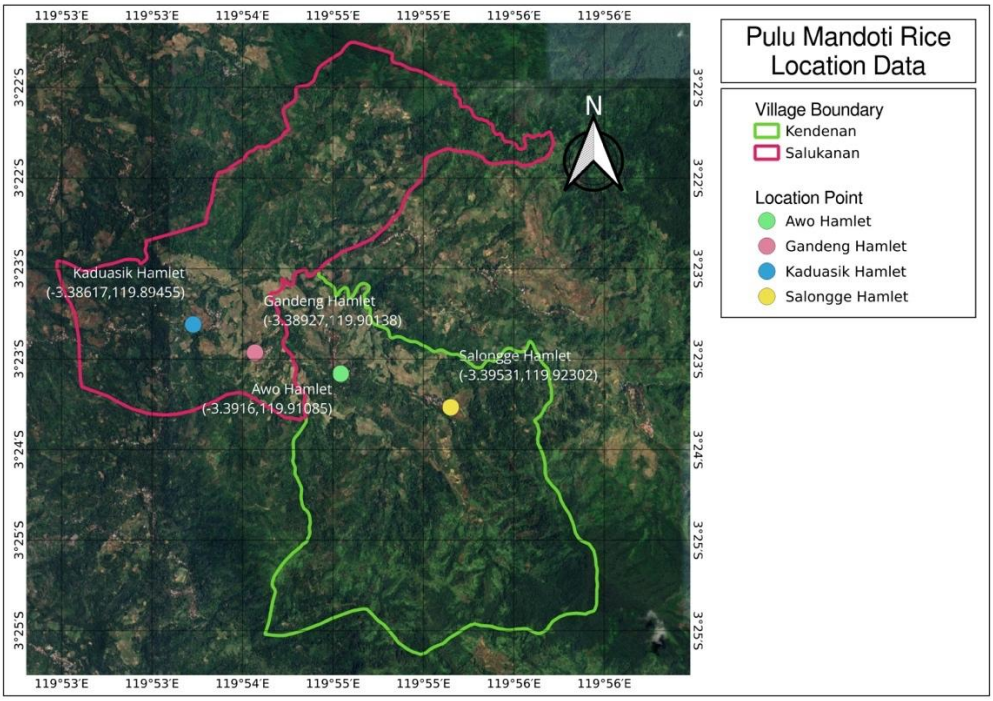


Fig. 1. Planting and sample location

The four sites are located within a relatively homogeneous agroclimatic zone, with a mean daily rainfall of 8.44 mm day^{-1}, an average air temperature of 23.38 °C, relative humidity of 86.76%, and atmospheric pressure of 93.17 kPa. Therefore, we assumed variation among locations reflected differences in elevation, soil characteristics, and micro-agroecological conditions rather than regional climatic variation.

We harvested Pulu Mandoti paddy during the same growing season from local farmers at each location, following the May–October 2024 planting period. After harvest, we dehulled the paddy using a standard rice milling machine to obtain milled white rice. The samples were then stored at 4 °C in airtight containers until volatile compound analysis.

2.2 Soil geochemical analysis

Composite soil samples were collected from the root-zone layer (0–20 cm depth) at each cultivation site and analyzed at the Soil Chemistry Laboratory, Soil Science Study Program, Faculty of Agriculture, Hasanuddin University, from October to November 2024. A total of 14 geochemical parameters were determined, including organic carbon (Walkley–Black method), total nitrogen (Kjeldahl method), C/N ratio, available phosphorus (Olsen method), exchangeable calcium (Ca), magnesium (Mg), and potassium (K), expressed in cmol(+) kg^{-1}, as well as sulfur (S) and the micronutrients boron (B), copper (Cu), iron (Fe), manganese (Mn), zinc (Zn), and molybdenum (Mo). In addition to the soil parameters, site-specific environmental variables, including elevation, rainfall, air temperature, relative humidity, and atmospheric pressure, were recorded as supporting environmental data.

2.3 Extraction and analysis of volatile compounds by HS-SPME–GC/MS

Volatile compound analysis was conducted at the Testing Laboratory of the Center for Rice Plant Engineering and Agricultural Modernization from July to August 2025 using the laboratory's internal method, IKM Kimia FR-01: Determination of Rice Flavor Profile based on Headspace Solid-Phase Microextraction Gas Chromatography Mass Spectrometry (HS-SPME–GC/MS). We weighed a 5 g portion of milled rice into a 20 mL SPME vial. We heated the sample at 90 °C for 60 min to establish headspace equilibrium while a 2 cm DVB/CAR/PDMS (divinylbenzene/carboxen/polydimethylsiloxane) fiber simultaneously extracted volatile compounds. This fiber is commonly used to extract volatile compounds spanning a broad range of polarities in food matrices.

Chromatographic analysis was performed using an Agilent 7890A gas chromatograph coupled to an Agilent 5975C XL EI/CI mass spectrometer. The SPME fiber was desorbed in the injection port at 250 °C for 5 min in splitless mode, with helium used as the carrier gas at a flow rate of 0.8 mL min^{-1}. Volatile compounds were separated using a

DB-Wax capillary column (30 m × 250 μm × 0.25 μm film thickness). The oven temperature program started at 40 °C and held for 0 min, then increased to 220 °C at 4 °C min^{-1} and held for 10 min. We maintained the GC–MS interface, ion source, and quadrupole temperatures at 250 °C, 230 °C, and 150 °C, respectively. Mass spectra were acquired over an *m/z* range of 29–550.

We tentatively identified volatile compounds by matching their mass spectra against the NIST14 Mass Spectral Library. Accordingly, we considered all compounds reported in this study tentatively identified because we assigned their identities based on mass spectral similarity and did not confirm them using authentic reference standards or retention indices. We expressed the relative abundance of each compound as the relative peak area (%) calculated from the peak area of the individual compound relative to the total chromatographic peak area.

2.4 Data analysis

Statistical analyses were performed on two datasets: (1) 14 soil geochemical parameters and (2) 23 volatile compounds consistently detected across all locations, representing the core volatilome, from a total of 172 annotated volatile compounds. All analyses were conducted using the Scikit-learn library in Python version 3.11. Before multivariate analysis, we log-transformed and Pareto-scaled the data. Pareto scaling is commonly applied in GC–MS-based metabolomic analyses to reduce the influence of high-variance variables while retaining biologically relevant information. (Ratnasekhar et al., 2020; Zhou et al., 2022).

Principal Component Analysis (PCA) was performed using the correlation matrix to minimize the influence of differences in variable scales. The statistical significance of each principal component was evaluated using a permutation test with 9,999 iterations, while 95% confidence intervals for the loading values were estimated using bootstrap resampling with 9,999 iterations (Jolliffe and Cadima, 2016).

Hierarchical cluster analysis was performed using Ward's method with Euclidean distance. To identify volatile compounds contributing to discrimination among cultivation locations, we performed Partial Least Squares–Discriminant Analysis (PLS-DA) using cultivation location as the class variable. We calculated Variable Importance in Projection (VIP) scores for each compound. We used a VIP threshold of ≥1.0 as a preliminary criterion for identifying discriminant compounds, consistent with approaches commonly applied in volatile metabolomics-based geographical authentication studies (Ratnasekhar et al., 2020; Asimi et al., 2022).

The associations between soil geochemical parameters and the relative abundances of volatile compounds were evaluated using Spearman's rank correlation analysis, with statistical significance set at $p < 0.05$.

Results and discussion

3.1 Soil geochemical characteristics at the four cultivation locations

The analysis of 14 soil geochemical parameters across the four Pulu Mandoti cultivation locations revealed substantial variation among sites (Table 1). Organic carbon content ranged from 0.88% in Kaduasik to 2.14% in Gandeng, while total nitrogen ranged from 0.09% in Kaduasik to 0.19% in Awo. The C/N ratio ranged from 10 to 16, indicating relatively similar levels of organic matter decomposition across the four locations. Available phosphorus (P_2O_5) ranged from 8.06 ppm in Kaduasik to 11.99 ppm in Gandeng.

The most pronounced differences were in metal micronutrient concentrations. Kaduasik exhibited substantially higher Cu (12.336 ppm) and Zn (21.047 ppm) concentrations than the other three locations, approximately 60–80 times and 17–27 times higher, respectively, than the lowest values recorded. These concentrations also exceeded the ranges of available Cu and Zn typically reported for uncontaminated tropical paddy soils (generally <2 ppm Cu and <5 ppm Zn). The elevated Cu and Zn concentrations may therefore reflect not only differences in soil fertility but also potential influences of local geological characteristics, such as metal-rich parent materials, or historical anthropogenic inputs, including residues from copper based fertilizers or pesticides. However, the present study did not directly evaluate these potential sources.

In contrast, Salongge exhibited the highest Fe (525.62 ppm) and Mn (45.62 ppm) concentrations. In contrast, Awo and Gandeng showed a relatively balanced nutrient profile, with higher levels of organic C, N, Ca, Mg, and K. Overall, the observed heterogeneity in soil geochemical characteristics provides important environmental context for evaluating their potential associations with the volatile compound profiles of Pulu Mandoti rice.

Table 1. Soil geochemical and agroclimatic characteristics at the four Pulu Mandoti cultivation locations

Parameter	Cultivation locations			
	Gandeng	Kaduasik	Awo	Salongge
C-organic (Walkley & Black, %)	2.14	0.88	1.83	1.69
N-total (Kjeldahl, %)	0.13	0.09	0.19	0.11
Rasio C/N	16	10	10	15
P_2O_5 available (Olsen, ppm)	11.99	8.06	11.63	8.75
Ca (cmol(+) kg^{-1})	3.46	1.68	4.57	0.82
Mg (cmol(+) kg^{-1})	1.32	0.85	0.75	0.60
K (cmol(+) kg^{-1})	0.53	0.15	0.54	0.54
S (%)	0.12	0.06	0.09	0.14
B (ppm)	0.196	0.810	0.225	0.756
Cu (ppm)	0.196	12.336	0.211	0.155
Fe (ppm)	265.32	41.025	314.15	525.62
Mn (ppm)	19.85	2.355	26.25	45.62
Zn (ppm)	1.225	21.047	0.795	2.510
Mo (ppm)	19.36	0.958	24.17	36.54
Rainfall (mm/day)	8.44	8.44	8.44	8.44
Air pressure (kPa)	93.17	93.17	93.17	93.17
Humidity (%)	86.76	86.76	86.76	86.76
Average temperature (°C)	23.38	23.38	23.38	23.38
Elevation (m a.s.l.)	867	750	965	1054

Source: Soil Chemistry Laboratory, Faculty of Agriculture, Hasanuddin University.
Note: Rainfall, air pressure, and humidity were relatively uniform across the four locations.

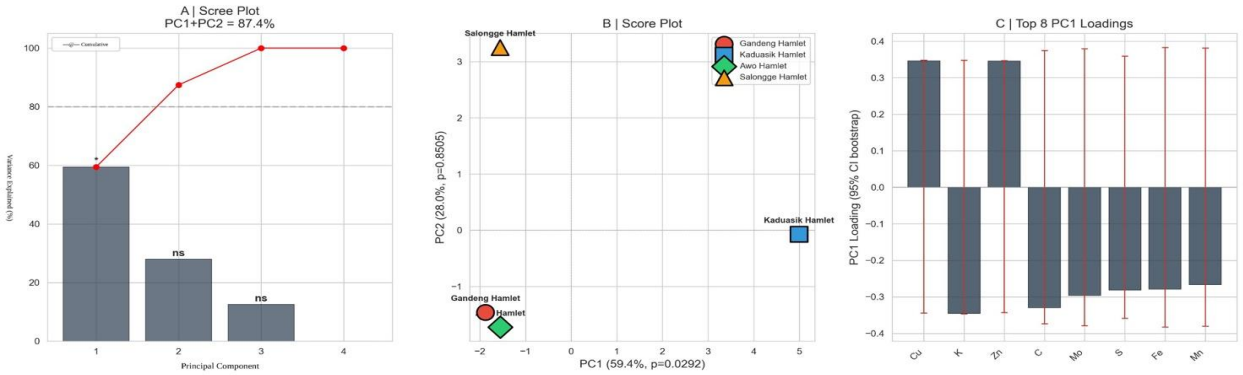


Fig. 2 Principal Component Analysis (PCA) of soil geochemical parameters. (A) Scree plot with significance based on a permutation test (*p<0.05); (B) PCA score plot; (C) Eight highest PC1 loadings with 95% bootstrap confidence intervals.

PCA of the 14 soil geochemical parameters yielded two principal components that cumulatively explained 87.44% of the total variance (PC1 = 59.43%; PC2 = 28.01%; Fig. 2A). The permutation test indicated that only PC1 was statistically significant (p = 0.030), whereas PC2 was not (p = 0.853), suggesting that the first principal component primarily captured the dominant structure in the dataset.

The PCA score plot (Fig. 2B) showed clear differentiation among the cultivation locations. Kaduasik was positioned on the positive side of PC1 (score = +4.99), largely associated with its high Cu and Zn concentrations, whereas the other three locations clustered on the negative side of PC1. Along PC2, Salongge was separated on the positive side (score = +3.25), primarily associated with its relatively high Fe and Mn concentrations.

The loading plot (Fig. 2C) indicated that PC1 represented a contrast between variables associated with organic nutrient status and metal micronutrients. Organic C, K, Mo, Fe, and Mn showed negative loadings, whereas Cu, Zn, and B showed positive loadings. This pattern was consistent with the correlation circle (Fig. 4), in which organic C, K, Mo, Fe, Mn, N, P_2O_5, Ca, and Mg formed a cluster of positively correlated variables. In contrast, Cu and Zn were positioned nearly orthogonally to this group. The orthogonal relationship suggests that the variation in Cu and Zn concentrations at Kaduasik may be relatively independent of the soil organic matter and nutrient related variables

represented in the PCA. Further investigation, including parent-material characterization and land-use history assessment, would therefore be required to determine whether this pattern reflects inherent site characteristics or potential anthropogenic influences. The heatmap summarizes the variation in soil geochemical parameter concentrations across the four cultivation locations (Fig. 3).

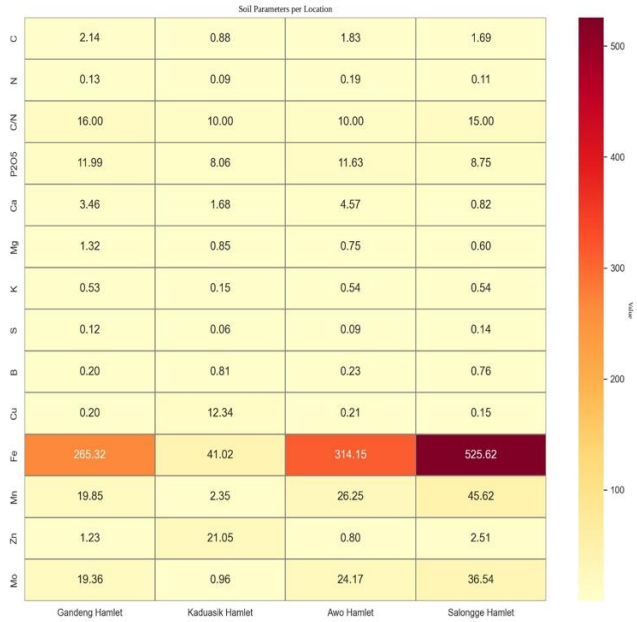


Fig. 3 Heatmap of soil geochemical parameter concentrations across the four planting sites. Red color intensity indicates higher values.

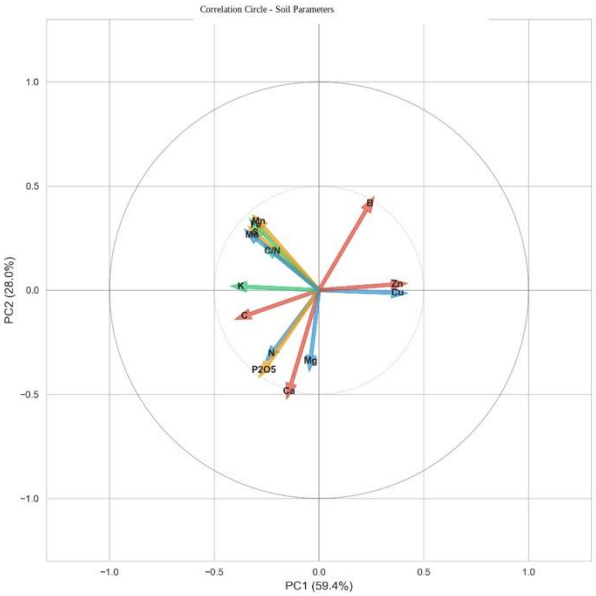


Fig. 4 Correlation circle of soil parameters on the PC1–PC2 plane. Vectors pointing in the same direction indicate a positive correlation; opposite directions indicate a negative correlation.

As shown in Fig. 3, the four cultivation locations exhibited contrasting soil geochemical profiles. Kaduasik had the highest Cu and Zn concentrations, whereas Salongge had the highest Fe, Mn, and Mo concentrations. Gandeng had the highest organic C and available P_2O_5 values, while Awo had the highest total N and Ca values (Table 1). These differences illustrate the edaphic heterogeneity among the study locations and provide context for exploring associations with volatile compound composition. Considering mineral information together with volatile profiles is consistent with the complementary analytical approach used by Du et al., (2018) to discriminate rice geographical origins. Their findings support this analytical rationale, but do not establish that the soil differences observed here caused the volatile differences.

3.2 Overall volatile compound composition of Pulu Mandoti rice

HS-SPME–GC/MS analysis identified 172 volatile compounds in Pulu Mandoti rice across the four cultivation locations (Table 2). The number of detected compounds varied by location, with Gandeng showing the highest number (91), followed by Awo (78), Kaduasik (71), and Salongge (62). Although Gandeng had the most detected compounds, Awo showed the highest total relative peak area. This finding indicates that compound richness and relative abundance are not necessarily directly proportional. In other words, a location may contain fewer detected compounds but may be dominated by a smaller number of compounds with substantially higher relative abundances. A similar pattern has been reported in other plant-based food matrices (Setyaningsih *et al.*, 2019). The HS-SPME–GC/MS chromatograms of Pulu Mandoti rice from Awo, Gandeng, Kaduasik, and Salongge are shown in Fig. 5A–D, respectively.

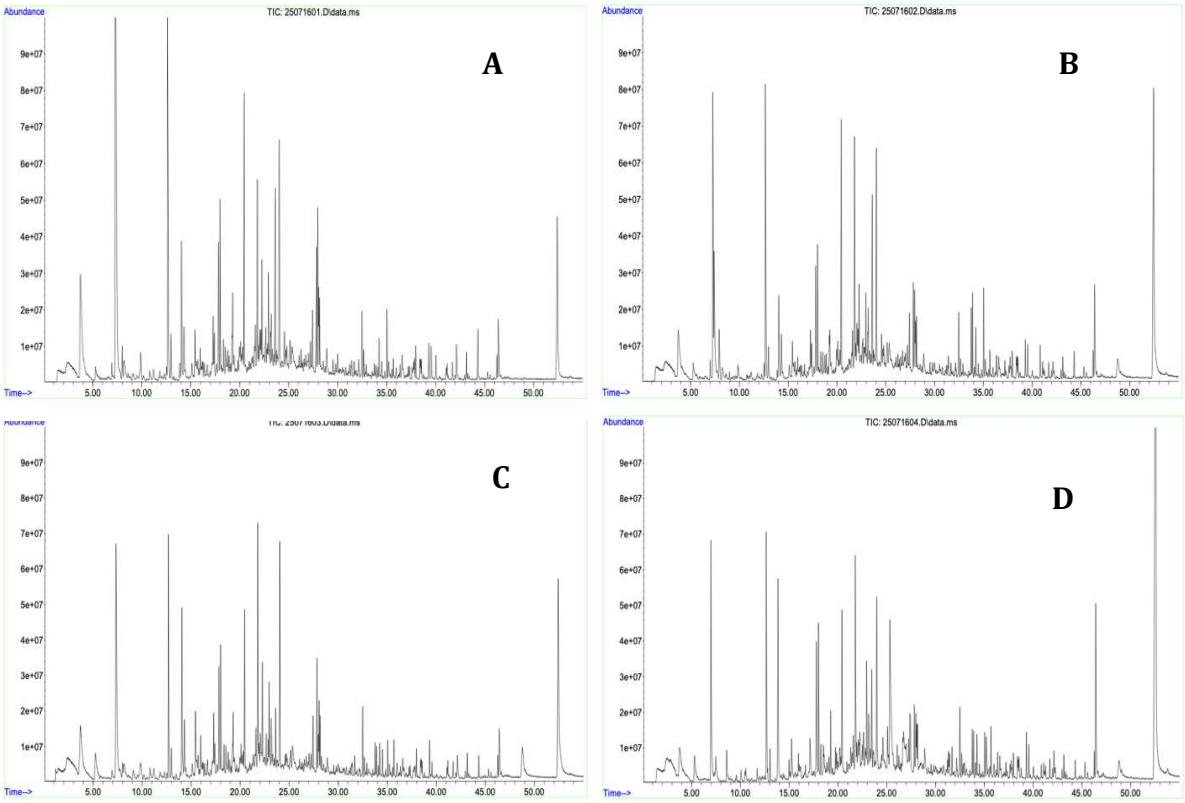


Fig. 5. HS-SPME–GC/MS chromatograms of volatile compounds in Pulu Mandoti rice at the four planting locations. (A) Awo; (B) Gandeng; (C) Kaduasik; (D) Salongge.

Figure 5 presents the HS-SPME–GC/MS chromatograms of Pulu Mandoti rice collected from Awo (A), Gandeng (B), Kaduasik (C), and Salongge (D). The chromatograms display multiple peaks distributed across the analytical retention-time range, illustrating the complexity of the extracted volatile mixtures. Several prominent peaks occur at broadly similar retention times among locations, whereas differences are apparent in peak intensity and the distribution of less prominent signals. These patterns are consistent with the presence of both shared volatile constituents and variation in volatile composition among the four cultivation locations. Nevertheless, similar retention times alone do not confirm compound identity, which requires interpretation of the corresponding mass spectra.

All identified volatile compounds were classified into eight chemical groups (G1–G8) based on their structural characteristics and functional groups (Table 2). Aldehydes (G2; 16 compounds) and alcohols (G4; 33 compounds) were the most dominant groups across all locations, consistent with volatile profiles previously reported for various aromatic rice cultivars (Kasote et al., 2021; Zhou et al., 2022). The aldehyde group accounted for approximately 7–17% of the total peak area, with the highest contribution observed in Kaduasik. In contrast, the alcohol group accounted for approximately 8–22% of the total peak area and reached its highest value in Awo. The terpene and sesquiterpene group (G5; 32 compounds) showed substantial variation among locations, with abundance in Awo more than twice that observed in Kaduasik. This variation suggests that the terpenoid biosynthetic pathway may be relatively sensitive to environmental conditions, as widely reported across various cereal species (Setyaningsih *et al.*, 2019).

Table 2 Classification of 172 Pulu Mandoti volatile compounds into eight chemical groups (G1–G8) with aroma descriptions and mean relative abundance (± SD, % peak area) at the four locations

Code	Group	Aroma description	No.	Awo Mean ± SD (n)	Gandeng Mean ± SD (n)	Kaduasik Mean ± SD (n)	Salongge Mean ± SD (n)
G1	Pyrrolines, pyridines & pyrazines	2-AP relatives/analogues-characteristic aromatic rice aroma markers	20	0.2568 ± 0.0994 (n=3)	0.1607 ± 0.1083 (n=10)	0.2158 ± 0.1122 (n=9)	0.1936 ± 0.1102 (n=6)
G2	Aldehydes	Major co-odorant: green, fatty, floral, caramel, vanilla aroma	16	1.3644 ± 1.2461 (n=8)	0.8659 ± 0.8236 (n=8)	1.7265 ± 1.4861 (n=9)	1.0287 ± 1.1609 (n=12)
G3	Ketones & lactones	Roasted, violet, caramel, coconut, jasmine, fruity aroma	37	0.5698 ± 0.3914 (n=13)	0.4645 ± 0.3439 (n=21)	0.4800 ± 0.2690 (n=12)	0.4258 ± 0.3031 (n=8)
G4	Alcohols	Earthy, mushroom, rose, floral, green, citrus aroma	33	1.2219 ± 1.3713 (n=18)	0.6047 ± 0.3846 (n=14)	0.9147 ± 0.6407 (n=13)	0.7374 ± 0.7993 (n=12)
G5	Terpenes & sesquiterpenes	Floral, herbal, citrus, spicy, woody, earthy aroma	32	1.0217 ± 0.9294 (n=15)	0.6732 ± 0.3536 (n=16)	0.6356 ± 0.5098 (n=9)	0.7372 ± 0.6043 (n=12)
G6	Odor-active esters	Fruity aroma (pineapple, pear, plum), jasmine, floral-balsamic	16	0.6078 ± 0.6974 (n=8)	0.5020 ± 0.4494 (n=11)	0.7123 ± 0.8593 (n=6)	0.7112 ± 0.6379 (n=3)
G7	Aromatic phenols & ethers	Clove, anise, spicy-warm, smoky aroma	11	0.5511 ± 0.4525 (n=6)	0.5792 ± 0.4277 (n=6)	0.5482 ± 0.3137 (n=7)	0.5495 ± 0.2008 (n=3)
G8	Furans & volatile organic acids	Buttery, popcorn, vinegar, cheesy, dairy aroma-oxidation & Maillard products	7	0.5988 ± 0.2414 (n=7)	0.3387 ± 0.1488 (n=5)	0.4508 ± 0.1944 (n=6)	0.6464 ± 0.3164 (n=6)
	Total		172	78	91	71	62

Source: primary data. Note: n = number of compounds detected within the group at that location.

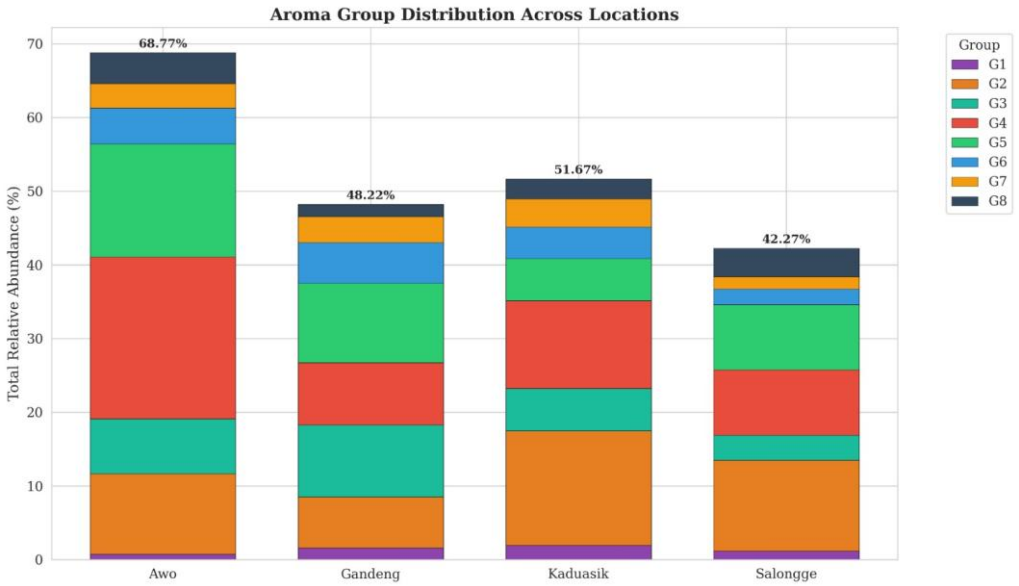


Fig. 6 Distribution of aroma groups (G1–G8) across the four Pulu Mandoti planting locations.

Examination of the relative abundances of individual volatile compounds (Fig. 6) revealed a clear hierarchy among the dominant volatile constituents. Nonanal (G2) was the most abundant compound across all cultivation locations, with relative peak areas ranging from 1.89% in Gandeng to 4.40% in Kaduasik. This straight-chain aldehyde is formed through the autoxidation or peroxidation of oleic acid and is generally associated with fatty, green, and citrus aroma notes. Several studies have also reported that nonanal may negatively affect the overall aroma perception of rice when present at relatively high concentrations (Li et al., 2024; Zheng et al., 2022).

Benzaldehyde (G2) was the second most abundant compound across all locations, with relative peak areas ranging from 2.32% to 3.25%. This compound is derived from phenylalanine degradation via the shikimic acid pathway and contributes almond-like and floral aroma notes. In addition to these two major compounds, several volatile compounds exhibited highly location-specific distribution patterns. (R)-3-cyclohexen-1-ol, 4-methyl-1-(1-methylethyl), reached relative abundances of 5.46% in Awo and 3.00% in Salongge but was not detected in either Gandeng or Kaduasik. In contrast, 2-octenal, 2-butyl was detected exclusively in Kaduasik, with a relative peak area of 2.94%, whereas an octahydronaphthalene derivative increased markedly in Awo, reaching 3.96%. These location-specific distribution patterns of individual volatile compounds provided the basis for sample discrimination in the multivariate analyses presented in the following section.

3.3 Unique location specific compounds as markers of chemical diversity among locations

In addition to relative abundance, information on the presence or absence of individual compounds at specific locations, particularly compounds detected exclusively at a single location (unique or location-specific compounds), provides an important additional layer of evidence supporting geographical authentication. Unlike continuous abundance data, binary presence–absence data are less affected by quantitative thresholds and may therefore provide more stable indicators of geographical differentiation (Asimi et al., 2022; Zhou et al., 2022). Of the 172 volatile compounds identified, 105 compounds (61%) were location-specific, being detected at only one of the four study locations. In contrast, the remaining compounds were detected at two or more locations (Table 3). The high proportion of location-specific compounds suggests substantial environmental plasticity in the volatile composition of Pulu Mandoti, thereby supporting the potential use of its volatile profile as a geographical fingerprint (Ratnasekhar et al., 2020; Tanaka et al., 2025).

Table 3 Number of specific compounds (detected at only one location) per chemical group across the four Pulu Mandoti planting locations

Code	Group	Total compounds	Awo	Gandeng	Kaduasik	Salongge	Total
G1	Pyrrolines, pyridines & pyrazines	20	0	7	6	2	15
G2	Aldehydes	16	1	1	2	3	7
G3	Ketones & lactones	37	6	14	4	2	26
G4	Alcohols	33	7	5	5	3	20
G5	Terpenes & sesquiterpenes	32	4	6	3	8	21
G6	Odor-active esters	16	2	6	2	0	10
G7	Aromatic phenols & ethers	11	2	2	2	0	6
G8	Furans & volatile organic acids	7	0	0	0	0	0
	Total	172	22	41	24	18	105

Source: Primary data, 2025

Note: Values in the location columns represent the number of compounds within that group detected only at that location (not present at the other three locations); Total compounds = cumulative number of location-exclusive compounds within that group across the four locations.

Table 3 summarizes the distribution of the 105 location-specific volatile compounds across the eight chemical groups. Gandeng contributed the largest number (41), followed by Kaduasik (24), Awo (22), and Salongge (18). Ketones and lactones (G3) accounted for the largest number of location-specific compounds (26), followed by terpenes and sesquiterpenes (G5; 21) and alcohols (G4; 20), whereas furans and volatile organic acids (G8) contributed none. These counts describe differences in compound occurrence among locations; they do not measure relative abundance or sensory contribution. The potential relevance of location-dependent volatile profiles to geographical authentication is supported by Asimi et al., (2022), who discriminated rice origins using VOC fingerprints and multivariate analysis.

However, compound occurrence alone cannot establish aroma importance: Li et al., (2024) combined GC–olfactometry, odor activity values, and sensory correlations to identify potentially characteristic rice volatiles. Thus, the location-specific compounds reported here are treated as candidates for further geographical and sensory validation.

Location-specific compounds were distributed heterogeneously across the four cultivation locations. The high proportion of location-specific compounds in Gandeng is noteworthy because this location did not dominate the relative abundance analysis or show clear group separation in the PCA and PLS-DA. This finding indicates that compositional richness and abundance represent two distinct dimensions that are not necessarily directly correlated. Thus, a location may show greater qualitative diversity in volatile compounds without quantitative dominance, as reported in studies of cereal volatiles from different production regions (Setyaningsih et al., 2019; Zhou et al., 2022).

At the chemical-group level, the distribution of location-specific compounds provides mechanistic information that complements the abundance patterns described in Section 3.2. Group G3 (ketones and lactones) contributed the most location-specific compounds, with 26 of its 37 members (70%) being location-specific; Gandeng had the highest number (14 compounds). In rice, ketones and lactones are generally formed through a combination of lipid oxidation pathways and nonenzymatic Maillard reactions during drying and postharvest storage. The formation of these compounds is known to be sensitive to postharvest conditions and to the composition of precursor fatty acids, which may vary according to the growing environment (Zheng et al., 2022; Tanaka et al., 2025).

In contrast, Group G8 (furans and volatile organic acids) contained no location-specific compounds, indicating that all members of this group were detected at least at two locations. This pattern is consistent with the relatively ubiquitous formation of furans through lipid oxidation and Maillard reactions, which may be less sensitive to site-specific edaphic conditions. Consequently, these compounds tend to be consistently formed in rice from different locations when exposed to similar postharvest conditions (Zheng et al., 2022; Li et al., 2024).

Group G1 (pyrrolines, pyridines, and pyrazines), which includes analogs or related compounds of 2-acetyl-1-pyrroline (2-AP), exhibited the second-highest proportion of location-specific compounds, with 15 of its 20 members (75%) being location-specific. Gandeng had the highest number of location-specific compounds in this group, with seven compounds. This finding complements the abundance analysis presented in Section 3.5 (Fig. 8). Although Kaduasik showed the highest overall abundance of Group G1, Gandeng exhibited greater compositional diversity of pyrroline, pyridine, and pyrazine derivatives. In contrast, Awo had no location-specific G1 compounds, although several members of this group were still detected as compounds shared with other locations (Table 2). This pattern indicates that high compound abundance does not necessarily accompany high compositional diversity, as observed in Kaduasik and Salongge. Conversely, Gandeng exhibited relatively lower overall abundance but greater compound diversity. These observations suggest that the growing environment may influence not only the accumulation of 2-AP and its related compounds but also the formation of various heterocyclic compounds derived from their transformation or degradation. This interpretation is consistent with the complexity of the proline-derived aroma biosynthetic pathway in rice, which involves multiple genes and enzymes (Xie et al., 2019; Wakte et al., 2016).

Group G5 (terpenes and sesquiterpenes) exhibited a different pattern. Salongge had the highest number of location-specific compounds, with eight of the 21 location-specific compounds in this group. Salongge was the highest-altitude site in the study, at 1,054 m a.s.l. Volatile terpenoid biosynthesis in rice proceeds through the mevalonate (MVA) and methylerythritol phosphate (MEP) pathways, which are catalyzed by various terpene synthase (OsTPS) enzymes. These pathways are known to be responsive to abiotic stresses, including increased UV-B radiation, which generally occurs at higher elevations (Shan and Jin, 2025). Therefore, the occurrence of location specific terpenoid compounds in Salongge may be mechanistically consistent with this environmental gradient. However, because the present study did not directly measure UV-B radiation intensity, this association remains a plausible hypothesis that future studies should verify.

Group G4 (alcohols) contributed the most location specific compounds in Awo, with seven compounds. This finding is consistent with the relative prominence of benzyl alcohol and various naphthalene derivatives previously identified as characteristic features of this location in Section 3.2. Meanwhile, Group G7 (phenols and aromatic ethers), which includes compounds such as guaiacol that are known to contribute to rice aroma characteristics (Li *et al.*, 2024) showed a relatively uniform distribution of location-specific compounds in Awo, Gandeng, and Kaduasik, with two compounds detected at each location, whereas no location-specific compounds from this group were detected in Salongge. This pattern may suggest that phenolic metabolism is less responsive to the altitudinal gradient than terpenoid biosynthesis, although this interpretation requires further experimental validation.

Overall, integrating location-specific compounds with relative abundance data and the multivariate analyses presented above provides further evidence that each Pulu Mandoti cultivation location has a distinct chemical fingerprint. These differences were reflected not only in the relative abundance of individual compounds but also in which compounds were present or absent at particular locations. The combination of quantitative data, represented by

relative abundance, and binary presence–absence data has increasingly been applied in volatile metabolomics studies for the geographical authentication of food products (Asimi et al., 2022; Zhou et al., 2022). In Pulu Mandoti, this integrated approach provides strong supporting evidence for chemical differentiation among cultivation locations. However, further validation is required before these patterns can serve as the basis for a geographical traceability system.

3.4 Multivariate discrimination and identification of candidate location-specific marker compounds

PCA of the 23 volatile compounds comprising the core volatilome (Fig. 7) yielded two principal components that explained a substantial proportion of the total data variance. The first principal component (PC1) explained 48.57% of the variance, and the second principal component (PC2) explained 33.89%, for a cumulative explained variance of 82.46%. The permutation test indicated that neither PC1 ($p = 0.174$) nor PC2 ($p = 0.357$) reached statistical significance at $\alpha = 0.05$. Therefore, PCA in the present study served as an exploratory approach to visualize sample distribution patterns and identify candidate discriminating variables, rather than as inferential evidence of statistically significant separation among the four populations. Nevertheless, the observed patterns remain biologically informative and provide a basis for hypotheses that should be further evaluated using a more adequate number of biological replicates (Jolliffe & Cadima, 2016; Ratnasekhar et al., 2020).

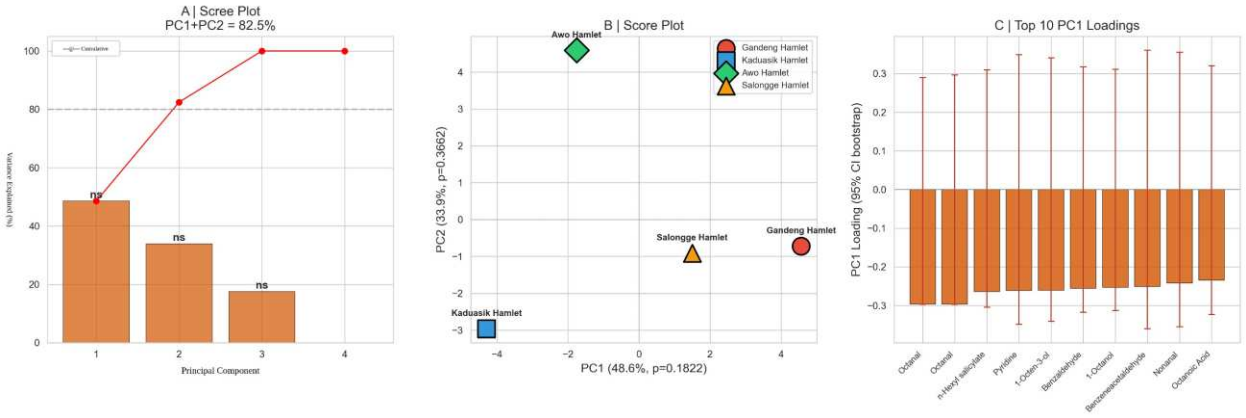


Fig. 7 Principal Component Analysis of core volatilome compounds. (A) Scree plot; (B) PCA score plot; (C) Ten highest PC1 loadings with 95% bootstrap confidence intervals.

The PCA score plot (Fig. 7B) still showed clear descriptive separation among the cultivation locations. Samples from Gandeng were positioned on the positive side of PC1 (score = +4.57), whereas Kaduasik (-4.30) and Awo (-1.76) were positioned on the negative side. Salongge occupied an intermediate position, with a PC1 score of +1.50. Along PC2, Awo was clearly separated on the positive side (score = +4.59), whereas Kaduasik was positioned on the negative side (-2.96). Loading analysis indicated that 2-phenylmethylene octanal, octanal, *n*-hexyl salicylate, pyridine, and 1-octen-3-ol were the major contributors to the negative side of PC1. In contrast, benzyl alcohol, 1,2-dimethoxybenzene, *n*-decanoate, a naphthalene derivative, and a benzoate ester contributed most strongly to the positive side of PC2.

To identify the compounds that contributed most to discrimination among cultivation locations, we performed PLS-DA using the four locations as discriminant classes. Given the limited number of classes and the absence of an independent validation dataset, we treated the PLS-DA model in the present study as a descriptive, exploratory approach with potential overfitting. Therefore, the resulting VIP scores should be regarded as a list of candidate marker compounds requiring further validation through biological replication and cross-validation rather than as definitive biomarkers (Ratnasekhar et al., 2020; Asimi et al., 2022). Based on this analysis, the compounds with the highest VIP scores were (R)-3-cyclohexen-1-ol, 4-methyl-1-(1-methylethyl) (VIP = 3.26), followed by nonanal (VIP = 2.38), 1,8a-dimethyl-7-(1-methylethenyl)octahydronaphthalene (VIP = 2.24), 2-butyl-2-octenal (VIP = 2.21), and butyl butanoate (VIP = 2.05).

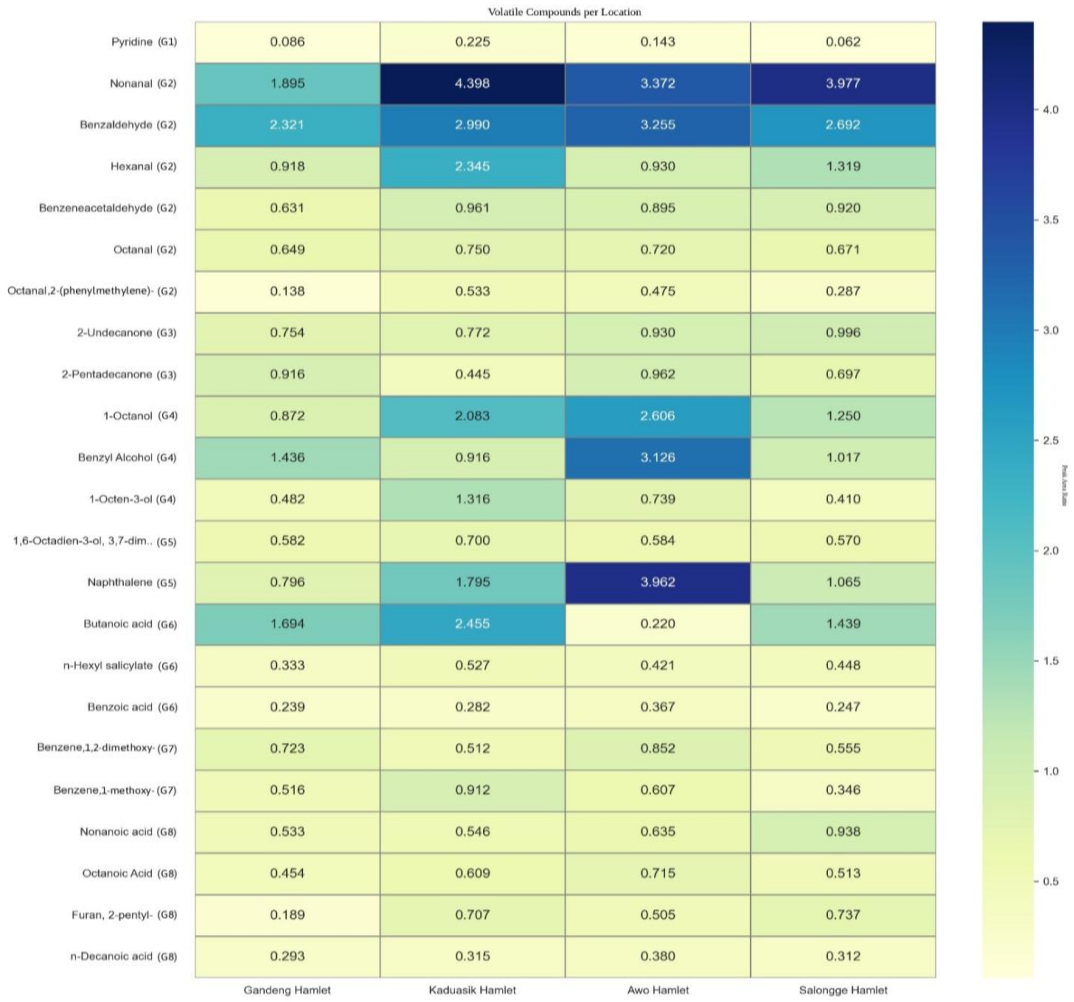


Fig. 8 Heatmap of the relative abundance of the 23 core volatilome compounds at the four planting locations. Higher blue intensity indicates higher values. Compound group codes (G1–G8) refer to Table 2.

The heatmap of the relative abundances of the 23 core volatilome compounds (Fig. 8) further supported the patterns observed in the PCA. High intensities of benzyl alcohol and naphthalene derivatives characterized Awo. In contrast, Kaduasik showed a predominance of nonanal, hexanal, butyl butanoate, and 1-octen-3-ol. Gandeng and Salongge exhibited more homogeneous patterns, with relatively lower intensities for most compounds. The consistency of patterns across PCA, PLS-DA, and heatmap analyses provides complementary evidence that the volatile profile of Pulu Mandoti exhibits location-specific characteristics and may serve as a chemical fingerprint for geographical origin authentication.

3.5 Group G1 (2-AP-related compounds) as potential indicators of aromatic rice aroma

The characteristic aroma of aromatic rice is generally associated with 2-acetyl-1-pyrroline (2-AP), a heterocyclic compound formed through proline- and ornithine-derived biosynthetic pathways involving the betaine aldehyde dehydrogenase (BADH2) enzyme. Mutations in the BADH2 gene have long been recognized as major genetic determinants of the aromatic phenotype in rice (Xie et al., 2019; Wakte et al., 2016). In addition to genetic control, 2-AP accumulation is also influenced by environmental conditions during grain filling, particularly temperature, plant water status, and nitrogen availability (Wei et al., 2017; Wakte et al., 2016).

Although Pulu Mandoti is recognized as an aromatic rice, we did not detect 2-acetyl-1-pyrroline in any samples analyzed using the untargeted GC–MS approach employed in this study. The absence of detectable 2-AP does not necessarily indicate that the compound is absent from Pulu Mandoti. Rather, this result may reflect analytical

limitations and 2-AP's physicochemical properties. The compound is highly volatile, readily oxidized, and unstable during drying, storage, milling, and sample preparation, which may cause substantial losses before analysis (Widjaja et al., 1996; Wakte et al., 2016). Moreover, the naturally occurring concentration of 2-AP in aromatic rice is generally very low (μg kg^{-1}) and may therefore fall below the detection limit of untargeted GC–MS approaches. This aligns with Chen *et al.*, (2021), who note that GC–MS methods have low sensitivity for low-concentration Volatile Organic Compounds (VOCs), leaving some VOCs undetected. As a result, this analysis tends to highlight high-concentration VOCs as the primary differentiating factors among samples. Consequently, many studies have used more sensitive methods, such as optimized targeted SPME–GC–MS, GC–MS/MS, or stable isotope dilution assays (SIDA), to quantify 2-AP (Bryant & McClung, 2011; Wakte et al., 2016).

Although this study did not detect 2-AP, it identified 20 compounds in Group G1, including pyrrolines, pyridines, and pyrazines. These compounds represent structural analogs, derivatives, or related compounds of 2-AP that may share biosynthetic connections through common precursors in proline and ornithine metabolism (Xie et al., 2019; Wakte et al., 2016). The presence of these compounds suggests that metabolic processes associated with the formation of aromatic rice volatiles may occur in Pulu Mandoti. However, this study did not detect the end product, 2-AP, under the analytical conditions used. Accordingly, Group G1 may serve as an indirect proxy for activity in aroma-related metabolic pathways, but it should not be interpreted as a quantitative substitute for 2-AP concentration.

Group G1 distribution across the four locations showed clear geographical variation (Table 2). Kaduasik and Salongge had the highest total relative abundances of G1 (0.22% and 0.19%, respectively), about twofold higher than in Gandeng (0.16%). Meanwhile, Awo exhibited the greatest compositional diversity within G1, with three G1 compounds detected and a mean relative abundance of 0.26% among the samples in which these compounds were detected. The identified G1 compounds included 2,4,6-trimethylpyridine, 1-(1H-pyrrol-2-yl)ethanone, 2,6-dimethylpyrazine, and 2,5-dimethylpyrazine. These compounds have been associated with roasted, nutty, and grain-like aroma characteristics that commonly accompany the characteristic aroma of aromatic rice and may contribute to the complexity of the volatile profile, although they are not direct substitutes for the popcorn- or pandan-like aroma produced by 2-AP (Hu et al., 2020; Xie et al., 2019).

From a plant physiological perspective, the formation of proline-derived heterocyclic compounds, including various 2-AP-related compounds, is generally influenced by mild abiotic stress conditions during grain filling. Water deficit, relatively low nighttime temperatures, and adequate nitrogen availability have been reported to enhance proline accumulation as both an osmolyte and a key precursor for the biosynthesis of aroma-related compounds (Xie et al., 2019; Luo et al., 2021; Wakte et al., 2016). Interestingly, Kaduasik, the lowest-elevation site (750 m a.s.l.), exhibited relatively high G1 abundance. This pattern suggests that, in addition to temperature, edaphic factors may also contribute to the activity of aroma-related metabolic pathways.

This interpretation is further supported by molecular studies indicating that micronutrients, particularly Zn, can modulate the expression of genes involved in 2-AP biosynthesis, including genes associated with metal homeostasis (Imran *et al.*, 2022). A recent review also suggested that micronutrient availability is among the agronomic factors influencing the accumulation of aroma compounds in rice, in addition to genetic factors, including BADH2, and environmental conditions (Guo *et al.*, 2026). However, the potential involvement of Cu and Zn at the Kaduasik site in the present study remains correlational. Further verification through targeted quantification of 2-AP, field-based microclimatic measurements, and reciprocal or common-garden experiments is needed to disentangle genetic, environmental, and crop-management effects.

The presence or abundance of 2-AP-related compounds cannot be directly translated into perceived aroma quality by consumers. The contribution of individual compounds to overall aroma perception depends on their odor thresholds, interactions among compounds within the food matrix, and non-additive olfactory perception mechanisms (Hu et al., 2020; Verma & Srivastav, 2020). Nevertheless, this study is the first to describe the distribution of 2-AP-related compounds in Pulu Mandoti rice across different cultivation locations. These findings provide an important basis for future studies integrating untargeted metabolomics with targeted 2-AP quantification to understand better aroma formation mechanisms in this endemic rice variety from Sulawesi.

3.6 Correlation between soil geochemistry and the volatile compound profile

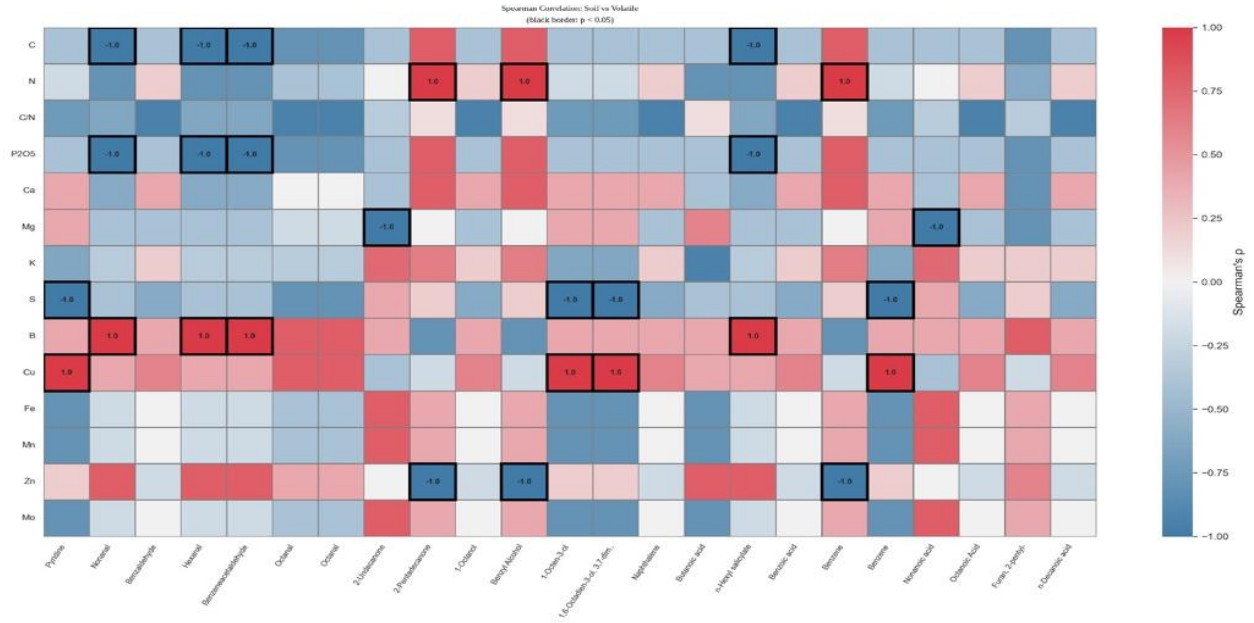


Fig. 9 Spearman correlation heatmap between soil parameters and volatile compounds. Black borders indicate correlations with $p<0.05$ at the site level (n=4).

Spearman correlation analysis (Fig. 9) revealed several patterns of association between soil chemical properties and the relative abundance of volatile compounds based on the mean values for each cultivation location. Before interpreting these results, it is important to emphasize the fundamental statistical limitation of this analysis. With only four observational units (n = 4), very high Spearman correlation coefficients, including $\rho = 1.00$, may arise simply from a perfect agreement in rank ordering among only 24 possible permutations (4!). Therefore, the correlation coefficients observed in this study cannot be interpreted as strong evidence of biological relationships, as they could be with a larger sample size. Accordingly, we treat all correlations presented below as descriptive, hypothesis-generating patterns rather than evidence of causal relationships.

Within this limitation, benzaldehyde tended to increase with increasing Fe, Mn, and Mo concentrations across the four locations. This association is biologically plausible because Fe and Mn serve as cofactors for enzymes in the phenylpropanoid and shikimate pathways, including phenylalanine ammonia-lyase (PAL), which converts phenylalanine into cinnamic acid derivatives that serve as precursors for benzaldehyde and benzyl alcohol. In addition, Mn is known to act as an activator of PAL and as a cofactor for 3-deoxy-D-arabino-heptulosonate-7-phosphate (DAHP) synthase, an early enzyme in the shikimate pathway (Lilay *et al.*, 2024). Nevertheless, this mechanistic interpretation requires confirmation through individual-sample analyses and direct measurements of PAL enzyme activity.

Nonanal and hexanal, two short- to medium-chain aldehydes generally produced through the peroxidation of unsaturated fatty acids, tended to increase with Cu and Zn concentrations but decrease under conditions with higher organic C, N, Ca, and Mg contents. This pattern is consistent with the general mechanism whereby redox-active transition metals, particularly Cu, can enhance the formation of reactive oxygen species (ROS), thereby accelerating membrane lipid peroxidation and generating aldehydes as secondary oxidation products. This mechanism has been widely reported in various plant species exposed to heavy-metal stress (Khan *et al.*, 2025). In the present study, Kaduasik, with the highest Cu (12.34 ppm) and Zn (21.05 ppm) concentrations, also showed the highest relative abundances of nonanal (4.40%) and hexanal (2.35%). However, because this condition was represented by only one location, the observed association cannot yet be considered a validated trend across a Cu and Zn concentration gradient. Further investigation using a broader range of metal concentrations or controlled pot experiments is therefore required before this relationship can be interpreted causally.

Butyl butanoate, a compound associated with a fruity aroma, tended to increase with Cu concentration but decrease with higher Fe content. As an ester formed through esterification reactions between short-chain fatty acids and alcohols, potentially mediated by endogenous esterases and epiphytic microbiota associated with harvested grain,

its formation likely reflects a combination of metabolic precursor availability and microbial activity. Therefore, variation in this compound's abundance is unlikely to be explained solely by soil geochemical factors.

In contrast, benzyl alcohol tended to increase in soils with higher Ca and Mg contents but decreased under high Cu concentrations. This pattern is consistent with the possibility that more balanced soil fertility conditions may support normal phenylpropanoid metabolism compared with metal-stress conditions.

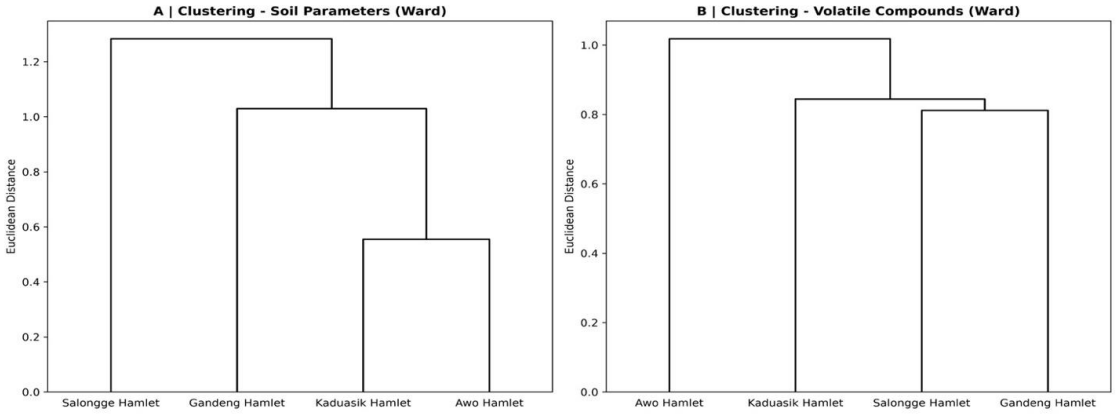


Fig. 10 Hierarchical clustering dendrogram (Ward's method, Euclidean distance) for (A) soil parameters and (B) volatile compounds.

Hierarchical cluster analysis (Fig. 10) provided an additional perspective on similarity among the cultivation locations. Based on the soil parameters, Gandeng and Awo formed a cluster with the smallest Euclidean distance, indicating relatively high geochemical similarity. Salongge joined the cluster at the subsequent clustering level, whereas Kaduasik formed a distinct branch, reflecting its distinctive soil geochemical characteristics, particularly its relatively high Cu and Zn contents. The dendrogram based on volatile compound profiles showed a topology generally similar to that derived from the soil parameters. The concordance between the two dendrograms suggests a potential association between soil geochemical characteristics and variation in the volatile compound composition of Pulu Mandoti rice, although this relationship remains descriptive.

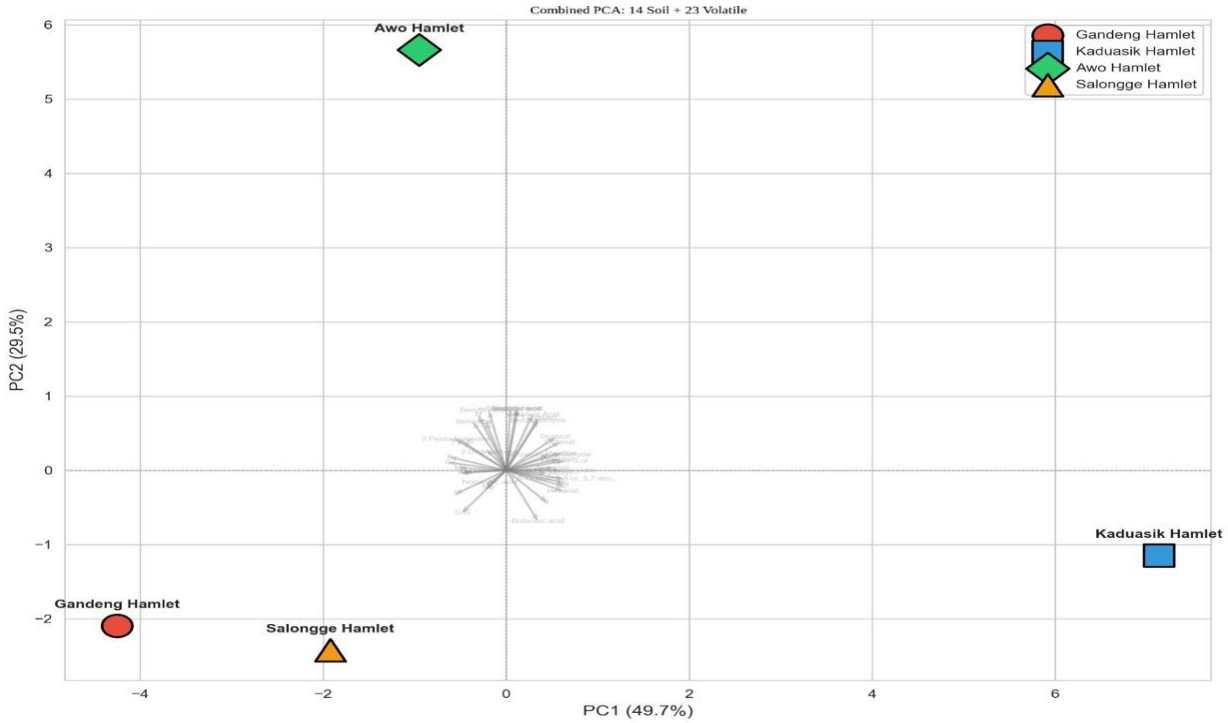


Fig. 11 Combined PCA biplot of 14 soil parameters and 23 volatile compounds (PC1 = 49.7%; PC2 = 29.5%).

The integrated PCA of 37 variables, comprising 14 soil parameters and 23 volatile compounds (Figure 11), produced a separation pattern consistent with the preceding analyses. Gandeng and Awo formed a closely positioned group; Kaduasik was clearly separated, whereas Salongge occupied an intermediate position. The loading vectors indicated that soil fertility-related parameters, such as organic C, K, Mo, Fe, and Mn, were associated with benzyl alcohol and various naphthalene derivatives. In contrast, Cu and Zn showed vector directions similar to those of nonanal, hexanal, and 1-octen-3-ol. Integrating these two datasets provided a coherent representation of location-specific chemical signatures. Nevertheless, applying these patterns as a traceability system still requires validation with more samples.

Overall, PCA, PLS-DA, Spearman correlation analysis, and hierarchical clustering indicated that the four Pulu Mandoti cultivation locations exhibited distinct soil geochemical characteristics and volatile profiles. Kaduasik was characterized by relatively high Cu and Zn contents, with a predominance of aldehydes such as nonanal, hexanal, and octanal, as well as 1-octen-3-ol. This pattern is consistent with the hypothesis that metal stress may enhance lipid peroxidation, although the present study could not directly confirm this mechanism. In contrast, Awo had relatively higher soil fertility and was dominated by benzyl alcohol, naphthalene derivatives, and 1-octanol. Gandeng showed geochemical characteristics similar to Awo but with lower abundances of most volatile compounds. Salongge displayed an intermediate profile, with the highest Fe and Mn contents and a relatively balanced volatile composition between the aldehyde and alcohol groups.

Interestingly, although Kaduasik and Salongge exhibited the highest abundances of Group G1 (2-AP-related compounds), Awo showed greater diversity within this aroma-related group. This finding suggests that Pulu Mandoti aroma may result from the interaction of multiple environmental and plant physiological factors and therefore cannot be explained by a single environmental gradient, such as soil fertility or the concentration of a particular metal.

These findings can be summarized in three main aspects. First, the results provide preliminary evidence that the volatile profile of Pulu Mandoti exhibits location-specific characteristics, supporting the development of a scientific basis for geographical indication systems. This finding is consistent with the increasing application of volatile fingerprinting and chemometric approaches for the authentication of agricultural products associated with geographical indications (Zhu, Zhu and Sun, 2023). The results also provide scientific support for local knowledge suggesting that the characteristic aroma of Pulu Mandoti is closely associated with its traditional cultivation area. However, the present study cannot test the claim that the characteristic aroma would diminish when Pulu Mandoti is cultivated outside Enrekang because it did not conduct a reciprocal or common-garden cultivation experiment. Second, identifying candidate compounds such as nonanal, benzyl alcohol, and naphthalene derivatives creates opportunities to develop chemical marker panels for product quality control and traceability systems. Nevertheless, these compounds require further validation using larger sample sizes and a broader range of cultivation locations. Third, the observed association between soil geochemical conditions and volatile profiles suggests that site-specific nutrient management may potentially contribute to maintaining or enhancing the characteristic aroma of Pulu Mandoti. However, because all analyses in this study were descriptive and based on only four cultivation locations, these findings cannot yet serve as a direct basis for agronomic recommendations and require further verification through controlled experiments.

4 Conclusion

This study shows that Pulu Mandoti aromatic glutinous rice has a volatile profile that differs by cultivation location within Baraka District, Enrekang Regency. We identified 172 volatile compounds: 23 formed the core volatilome, and 105 (61%) were location-specific, indicating a distinctive volatile fingerprint at each location. Multivariate analysis consistently separated volatile composition patterns among locations and identified several candidate marker compounds. At the same time, the distribution of the 2-AP analog group suggested variation in the aroma metabolic pathway, even though 2-acetyl-1-pyrroline (2-AP) itself was not detected.

Integrating the volatile profile with soil geochemical characteristics suggests that edaphic variation is likely associated with differences in the volatile compound composition of Pulu Mandoti. Although this relationship still requires validation through targeted 2-AP quantification and a larger sample size, these results provide a scientific basis for developing geographical authentication and traceability systems and for preserving Pulu Mandoti rice aroma quality.

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