



Visualisation of *Phyllanthus emblica* L. quality using E-nose, HS-SPME/GC-MS, and spectrophotometric methods with chemometrics

X. Liu^{1,2*} , Y. Li^{1*} , J. Chen¹, D. He^{1,2}, H. Li¹ and K. Wu^{1,2}

¹ School of Chemical Engineering and Light Industry, Guangdong University of Technology, Guangzhou 510006, China

² Guangdong Provincial Key Laboratory of Plant Resources Biorefinery, Guangzhou, China

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ABSTRACT

This paper provides a rapid method coupled with chemometrics to visualise PEL quality of eight regions. The contents of mineral elements, Vitamin C (Vc), and colour parameters were measured using spectrophotometric methods. The volatile substances were determined by electronic nose (E-nose) and headspace solid phase micro-extraction with gas chromatography-mass spectrometry (HS-SPME/GC-MS). Chemometric analyses were employed to visualise the sample distribution according to the geographical origin. The colour parameters, Vc, and mineral contents of PEL from diverse origins were significantly different ($P < 0.05$). A total of 25 volatile organic compounds (VOCs) were identified from PELs, with the highest percentage of components being ethyl acetate. The combination of HS-SPME/GC-MS and E-nose can properly characterise PEL samples. Therefore, the results of this exploratory work highlight the possibility of discriminating PEL from different regions.

KEYWORDS

Phyllanthus emblica L. (PEL), geographical origin, spectrophotometry, HS-SPME/GC-MS, E-nose, chemometrics

* Corresponding authors. E-mail: jumper45@sina.com, 904126539@qq.com

1. INTRODUCTION

Phyllanthus emblica L. (PEL) is a nutritious fruit found in subtropical and tropical regions such as India, Indonesia, and China, known for its medicinal properties (Saini et al., 2022). PEL, which has been traditionally used in the production of beverages or consumed as fresh fruit, has become increasingly popular in recent years (Sharma et al., 2022). Raw materials have a great impact on the quality of fruit juice products that consumers care about, such as colour (Munera et al., 2018), nutrients (Oldoni et al., 2022) and flavour (Li et al., 2017), thus the selection of high-quality raw materials is particularly important (Wu et al., 2021). The discrimination of raw materials using the tested parameters in combination with chemometric methods is an effective strategy (Wistaff et al., 2021). Moreover, Vitamin C (Vc) is a valuable nutrient and measured as one of the important parameters for product quality control of fresh fruits (Chikhale et al., 2021). In addition, the mineral composition analysis (Jandric et al., 2021) of PEL is helpful to explore its nutritional value as a food product, and can be used for its characterisation and geographical discrimination (Bin et al., 2022). Undoubtedly, the elemental composition of PEL fruits is influenced by several factors, such as geographical origin, variety and growing conditions. The mineral profiles of agricultural products can be used as authentic markers to determine their geographical origin.

In recent years, electronic nose (E-nose) (Kovács et al., 2010) and headspace solid phase micro-extraction with gas chromatography-mass spectrometry (HS-SPME/GC-MS) have been widely used for the analysis of fruit flavour components and separating products of different origins (Rocchi et al., 2019). In previous study, the characteristic aroma of Chinese PELs from Guangdong and Yunnan origin were determined, with the analysis of volatile organic compounds (VOCs) using E-nose and SPME/GC-MS (Huang et al., 2022).

The aim of this study was to provide a rapid method coupled with chemometrics to visualise PEL quality of eight regions. Principal component analysis (PCA) was performed to characterise the mineral composition as well as Vc and CIELAB parameters of PELs growing in eight regions of China. The main aroma substances in PELs were investigated by the E-nose and HS-SPME/GC-MS methods. Linear discriminant analysis (LDA) was used to evaluate the effectiveness of the methods for the detection and identification of the samples.

2. MATERIALS AND METHODS

2.1. Chemicals

Standard calibration curves were plotted for each mineral using standard minerals obtained from the Macklin Chemical Company, China. The standard substances of potassium, calcium, magnesium, copper, manganese, and zinc were potassium chloride, calcium carbonate, magnesium oxide, copper sulphate pentahydrate, manganese powder, and zinc oxide, respectively. All reagents were analytically pure.

2.2. *Phyllanthus emblica* L. sample

In this study, the PEL fruits were harvested at the recommended harvest times (September to November in 2021). The geographical locations of the sampling point are shown in Table 1.



Table 1. The geographical origins of the samples

Batch	Origin	East longitude	North latitude	Altitudes (m)
QUZ	Quanzhou	118.58	24.90	10
ZZ	Zhangzhou	117.66	24.51	20
ST	Shantou	116.70	23.37	18
PZH	Panzhuhua	101.71	26.58	1,400
YX	Yuxi	102.54	24.35	1,800
DL	Dali	100.24	25.59	1,976
QZ	Qinzhou	108.62	21.96	250
DZ	Danzhou	109.57	19.51	100

2.3. Colour parameters

Colour difference parameters are measured using the NS800 spectrophotometer (3NH, Shenzhen, China). The CIELAB colour scale was used to measure the L^* (lightness), a^* (redness/greenness), and b^* (yellowness/blueness) parameters (Patsilnakos et al., 2018).

2.4. Analysis of vitamin C

Fresh fruit samples were treated with a stabilising buffer solution before filtration, and 2,6-dichloroindophenol solution was added. Subsequently, the absorption was measured at 520 nm using a visible spectrophotometer (Jinghua, Shanghai, China). The vitamin C (Vc) content was expressed as mg g^{-1} fresh weight (FW) (Raghu et al., 2007).

2.5. Analysis of minerals

Enucleated PEL was ashed in a muffle furnace (Marit, Wuxi, China) at 550 °C for the separation of minerals from the plant matrix. After ashing and properly diluting, the ashed sample was sucked into an air-acetylene flame to burn the elements into the atomic components, and then detected by atomic absorption spectrophotometry (Model-AA-6880, Shimadzu, Tokyo, Japan) (Gonçalves et al., 2022).

2.6. E-nose analysis

The aroma of PEL from eight origins was measured with PEN 3.0 E-nose (Airsense Analytics GmbH, Schwerin, Germany). The samples (1 g) were placed in 20 mL headspace vials and measured after equilibration in a 45 °C water bath for 30 min. The measurement conditions were: washing time 120 s, reset time 5 s, pre-injection time 5 s, carrier gas flow rate 600 mL min^{-1} , and sample measurement time 80 s (Liu et al., 2018).

2.7. HS-SPME/GC-MS analysis

The extraction and analysis of volatile organic compounds (VOCs) were carried out under the published experimental protocol (Pico et al., 2022) with some modifications. PEL sample (1.5 g) was added into a 20 mL headspace vial. The headspace vial was then sealed with a screw cap with a PTFE silicon gasket, and a SPME needle was inserted. The extraction temperature was 35 °C



and the VOCs were absorbed for 30 min. The SPME needle was then inserted into the GC injector and the VOCs were detected by GCMS-7890-5975C (Agilent, USA). The carrier gas was He at a flow rate of 1.5 mL min^{-1} . The temperature program was as follows: $50 \text{ }^\circ\text{C}$ for 10 min; increase to $70 \text{ }^\circ\text{C}$ at a rate of $5 \text{ }^\circ\text{C min}^{-1}$; increase to $140 \text{ }^\circ\text{C}$ at a rate of $4 \text{ }^\circ\text{C min}^{-1}$; hold for 1 min; increase to $180 \text{ }^\circ\text{C}$ at a rate of $4 \text{ }^\circ\text{C min}^{-1}$; hold for 1 min; increase to $250 \text{ }^\circ\text{C}$ at a rate of $5 \text{ }^\circ\text{C min}^{-1}$; hold for 5 min. The temperature of the quadrupole and ion source was $250 \text{ }^\circ\text{C}$. The ion source was operated in electron impact (EI) mode at 70 eV. The full scan mode was applied across the m/z range of 40–400. In this study, unknown volatile compounds were qualitatively analysed by comparing NIST 17S software data.

2.8. Statistical analysis

Descriptive statistics were performed for all variables using SPSS 22.0 software (SPSS Inc., Chicago, USA). The differences between the groups were examined using a one-way ANOVA analysis of variance ($P < 0.05$). The graph was drawn from origin 2018. PCA was conducted using the Biozeron Cloud Platform (<http://www.cloud.biomicroclass.com/CloudPlatform>).

3. RESULTS AND DISCUSSION

3.1. Colour parameters and vitamin C content of PEL

The CIELAB data, obtained by the colorimetric analyses of the PEL samples were shown in Table 2. The colour parameters of PEL fruits from different sources were obviously different. The luminance L^* ranged from 50.51 to 59.75, and the L^* values of QUZ, ZZ, YX, and QZ samples were significantly higher than those for the other groups. Colour parameter a^* had negative values for all PEL fruits analysed, with a range from -2.53 to -5.66 . For the b^* values, a wide range from 6.61 to 19.91 was also observed in the studied samples (Munera et al., 2018).

The range of vitamin C content of the PELs used in the study was $5.63\text{--}21.55 \text{ mg g}^{-1}$ fresh weight (FW). Compared to the varieties of Thai (2.15 mg g^{-1} FW) (Kubola et al., 2011) and Indian ($2.07\text{--}4.69 \text{ mg g}^{-1}$ FW) (Raghu et al., 2007), the PELs of China investigated in this study had a substantially higher vitamin C content. Hence, for vitamin C, as one of the nutritional components of PEL, there were marked differences from diverse origins.

3.2. Mineral content of PEL

The macronutrient contents of potassium (K), calcium (Ca), and magnesium (Mg) in the fruits of eight PEL varieties cultivated in China are shown in Table 2. Potassium was the most abundant mineral element in all PEL samples. However, the K values recorded in the analysed samples ($31.92\text{--}90.94 \text{ mg/100 g FW}$) were lower than the value reported by Judprasong et al. (2013) (151 mg/100 g FW). Ca content of PEL varieties ranged from 33.34 to $72.73 \text{ mg/100 g FW}$. The YX species had the highest Mg content ($16.48 \text{ mg/100 g FW}$), while the lowest content (6.98 mg/100 g FW) was observed in the QZ species.

The contents of micromineral components copper (Cu), manganese (Mn), and zinc (Zn) in the fruits of eight PEL varieties produced in China are shown in Table 2. Mn was the most abundant minor element at $195.89\text{--}5,884.00 \text{ } \mu\text{g/100 g FW}$, followed by



Table 2. Colour parameters, vitamin C content, and mineral content of the eight varieties of *Emblica* fruits from China

Origin	Unit	Production area							
		QUZ	ZZ	ST	PZH	YX	DL	QZ	DZ
L*		58.01 ± 0.37 ^a	58.42 ± 0.95 ^a	51.50 ± 0.32 ^b	51.60 ± 3.78 ^b	59.75 ± 0.16 ^a	50.51 ± 1.73 ^b	56.73 ± 1.79 ^a	50.75 ± 1.42 ^b
a*		-4.08 ± 0.25 ^b	-2.53 ± 0.21 ^a	-5.30 ± 0.31 ^c	-3.66 ± 0.26 ^b	-5.46 ± 0.12 ^c	-4.10 ± 0.27 ^b	-5.66 ± 0.29 ^c	-2.86 ± 0.94 ^a
b*		11.61 ± 0.11 ^c	6.61 ± 0.37 ^d	13.82 ± 0.30 ^{bc}	13.65 ± 2.19 ^{bc}	19.91 ± 3.26 ^a	13.99 ± 0.97 ^{bc}	16.34 ± 0.69 ^b	12.35 ± 2.22 ^c
Vc	mg g ⁻¹	11.61 ± 1.02 ^b	6.96 ± 0.39 ^c	11.87 ± 0.81 ^b	21.55 ± 1.61 ^a	5.63 ± 0.75 ^c	7.43 ± 0.55 ^c	6.95 ± 1.81 ^c	6.59 ± 1.84 ^c
K	mg/100 g	36.41 ± 0.41 ^f	39.54 ± 0.81 ^e	31.92 ± 0.38 ^g	54.07 ± 1.49 ^c	88.42 ± 1.82 ^b	90.94 ± 1.52 ^a	54.88 ± 0.40 ^c	51.26 ± 0.61 ^d
Ca	mg/100 g	43.18 ± 0.69 ^e	33.34 ± 0.26 ^h	48.84 ± 0.45 ^d	67.52 ± 0.62 ^b	72.73 ± 0.98 ^a	61.61 ± 0.54 ^c	39.78 ± 0.47 ^g	40.73 ± 0.23 ^f
Mg	mg/100 g	7.75 ± 0.04 ^{de}	7.03 ± 0.72 ^f	8.57 ± 0.75 ^e	9.72 ± 0.46 ^c	16.48 ± 0.07 ^a	12.42 ± 0.02 ^b	6.98 ± 0.80 ^f	8.08 ± 0.08 ^e
Cu	µg/100 g	329.57 ± 3.18 ^f	374.77 ± 2.16 ^d	436.91 ± 2.84 ^b	627.83 ± 0.70 ^a	370.53 ± 1.08 ^d	339.93 ± 3.35 ^e	431.26 ± 1.77 ^c	271.88 ± 4.63 ^g
Mn	µg/100 g	4,076.17 ± 39.68 ^b	5,884.00 ± 7.90 ^a	544.44 ± 15.11 ^g	195.89 ± 20.11 ^h	1,923.39 ± 18.95 ^e	3,954.40 ± 7.90 ^c	1,096.95 ± 26.65 ^f	2,309.28 ± 36.61 ^d
Zn	µg/100 g	5.98 ± 0.40 ^h	15.78 ± 0.57 ^d	11.40 ± 0.18 ^g	12.03 ± 0.28 ^f	20.03 ± 0.48 ^c	13.65 ± 0.18 ^e	22.18 ± 0.15 ^b	29.67 ± 0.15 ^a

Vc: Vitamin C; Values (mean ± SD, $n = 3$) in the same line followed by a different letter are significantly different ($P < 0.05$).



Cu (271.88–627.83 $\mu\text{g}/100\text{ g FW}$) and Zn (5.98–29.67 $\mu\text{g}/100\text{ g FW}$). Substantially, the content of the analysed element showed a wide range of variation, which is a result of the geographical origin of PELs.

3.3. PCA of samples from different regions of PEL by colour parameters, vitamin c, and mineral content

Figure 1 displays the distributions of the first two principal components established by the PCA, depicting the cumulative 37.07% and 26.66% variance contributions, respectively. Clearly, the formation of eight groups can be perceived. The PCA plot demonstrated the differences of PELs from eight production areas in terms of their colour parameters, Vc, and mineral elements content. These results suggested that the geographical traceability of PELs in China is possible based on their physicochemical properties (Karabagias et al., 2017).

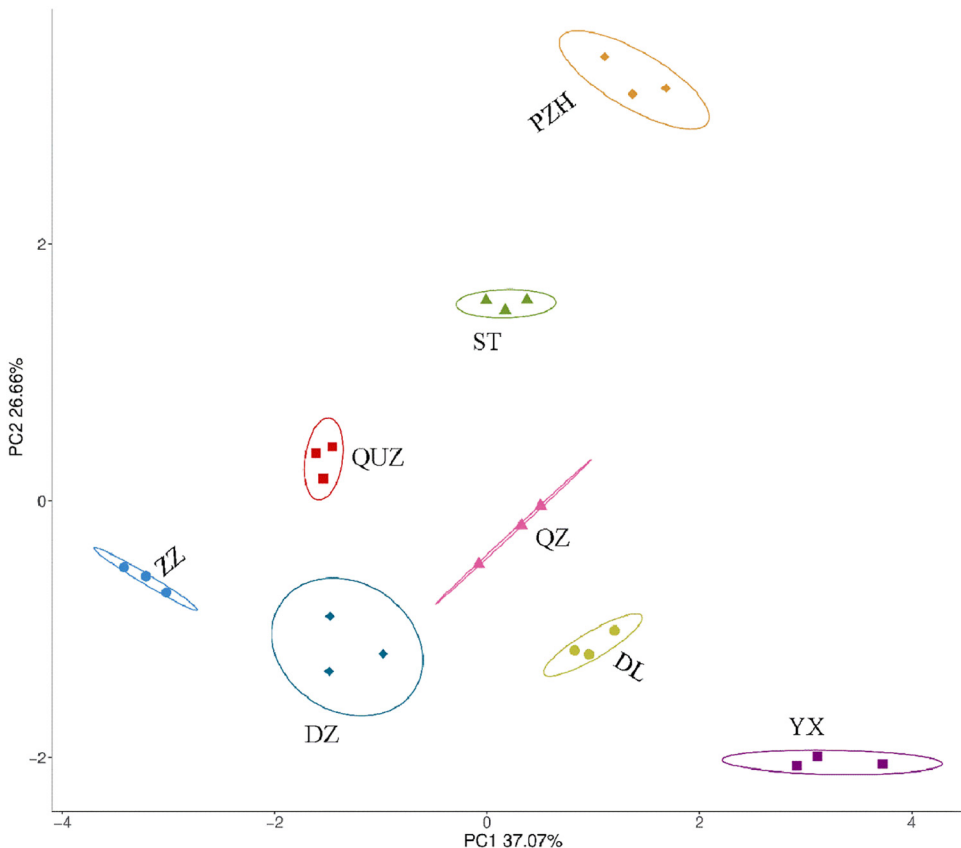


Fig. 1. Principal component analysis based on the colour parameter, vitamin C and mineral contents of PEL of different origin



3.4. E-nose data of PEL

The CA, LDA, and PCA analysis results of the E-nose were as follows. Based on the significant e-nose response of W5S, W1W, and W2W to PEL (Fig. 2A), cluster analysis (CA) was utilised to describe the variations in the aroma characteristics of PEL from different sources. From Fig. 2B, it can be seen that the aroma characteristic of PELs of QUZ, PZH, YX, and DL were similar. Since LDA maximises the interclass variance and minimises the intraclass variance, LDA method was used for the classification of the eight samples. The contributions of variance for LD1 and LD2 were 65.50% and 20.84%, respectively (Fig. 2C). The corresponding distances of the eight samples showed that the E-nose could discriminate PEL fruits from different sources. The distributions of the first two principal components identified by the PCA described a cumulative 97.40% and 2.02% of the variance contribution, respectively (Fig. 2D). The corresponding distances of the eight samples showed that the E-nose could discriminate PEL fruits from different sources.

3.5. Volatile compounds of PEL

In comparison with the NIST 17.0 library, a total of 25 VOCs was identified based on retention time, elution order, and other indicators as shown in Table 3. To visualise the situation, bar graphs were created based on the percentage data of volatile organic compound contents of the eight PEL fruits (Fig. 3).

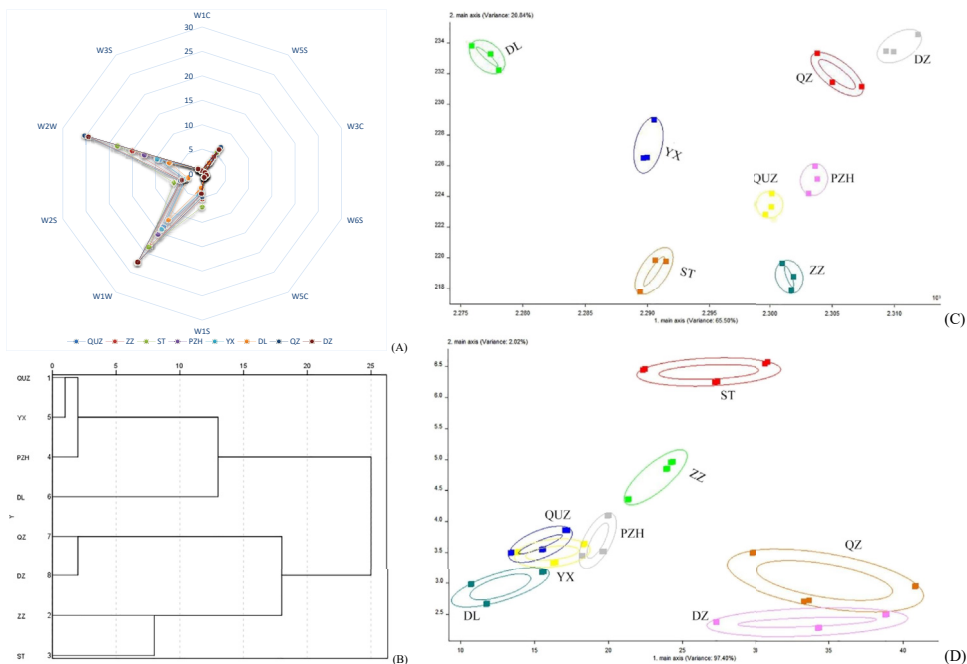


Fig. 2. Radar chart (A), cluster analysis (B), linear discriminant analysis (C), and principal component analysis (D) of the E-nose response data



Table 3. HS-SPME/GC-MS determination of volatile compounds in *Embllica* fruits of different origin

No	Volatile compounds (%)	QVZ	ZZ	ST	PZH	YX	DL	QZ	DZ
Esters									
1	Ethyl acetate	26.58 ± 1.39 ^e	31.04 ± 2.65 ^{de}	39.08 ± 6.53 ^{bcd}	33.81 ± 2.82 ^{cde}	40.60 ± 6.89 ^{bc}	35.59 ± 3.54 ^{bcd}	44.29 ± 6.87 ^b	55.63 ± 4.09 ^a
2	Isoamyl acetate	0.23 ± 0.01 ^c	0.63 ± 0.02 ^b	0.15 ± 0.05 ^c	2.72 ± 0.36 ^a	nd	nd	0.02 ± 0.00 ^c	nd
3	2-Methylbutyl acetate	nd	nd	nd	nd	nd	nd	nd	0.12 ± 0.00
4	Amyl acetate	0.47 ± 0.04 ^{cd}	1.16 ± 0.21 ^b	0.69 ± 0.07 ^{cd}	nd	2.14 ± 0.37 ^b	2.67 ± 0.33 ^b	nd	5.27 ± 0.95 ^a
5	Ethyl hexanoate	0.46 ± 0.08 ^b	0.70 ± 0.02 ^a	nd	0.14 ± 0.02 ^d	nd	nd	0.29 ± 0.07 ^c	0.15 ± 0.01 ^d
6	Cis-3-hexenyl acetate	27.48 ± 2.16 ^a	12.87 ± 1.02 ^b	nd	1.83 ± 0.10 ^c	nd	28.25 ± 2.66 ^a	nd	nd
7	4-Hexen-1-ol, 1-acetate	nd	nd	7.36 ± 0.76	nd	nd	nd	nd	nd
8	Trans-3-hexenyl acetate	nd	nd	nd	nd	8.28 ± 1.10 ^a	nd	nd	4.66 ± 0.72 ^b
9	Hexyl acetate	1.70 ± 0.12 ^c	12.62 ± 1.41 ^a	6.47 ± 0.60 ^b	1.07 ± 0.21 ^c	nd	nd	nd	0.78 ± 0.23 ^d
10	Trans-2-hexenyl acetate	nd	nd	7.02 ± 0.47 ^b	5.64 ± 1.03 ^c	nd	nd	nd	23.43 ± 1.06 ^a
11	Methyl benzoate	nd	nd	nd	0.22 ± 0.03	nd	nd	nd	nd
12	Ethyl benzoate	nd	nd	nd	2.69 ± 0.17	nd	nd	nd	nd
Alcohols									
13	Ethyl alcohol	0.84 ± 0.05 ^d	1.55 ± 0.14 ^c	3.60 ± 0.15 ^b	nd	nd	0.26 ± 0.05 ^e	5.09 ± 0.08 ^a	nd
Hydrocarbons									
14	Styrene	nd	nd	nd	nd	0.26 ± 0.01 ^b	nd	1.95 ± 0.46 ^a	nd
15	Alpha-Pinene	0.68 ± 0.06 ^a	0.28 ± 0.02 ^c	0.14 ± 0.01 ^{ef}	0.22 ± 0.00 ^{cd}	0.40 ± 0.08 ^b	0.16 ± 0.04 ^{de}	0.07 ± 0.01 ^f	0.25 ± 0.06 ^c
16	Sabinene	nd	0.15 ± 0.03 ^a	0.05 ± 0.01 ^b	nd	nd	nd	nd	0.07 ± 0.02 ^b
17	Beta-Pinene	0.51 ± 0.07 ^a	0.11 ± 0.01 ^d	nd	0.23 ± 0.07 ^c	nd	nd	nd	0.40 ± 0.14 ^b
18	<i>p</i> -Cymene	7.26 ± 0.14 ^a	5.27 ± 0.19 ^b	0.92 ± 0.19 ^e	1.07 ± 0.08 ^e	2.75 ± 0.38 ^c	1.60 ± 0.47 ^d	0.47 ± 0.16 ^f	0.35 ± 0.08 ^f
19	D-Limonene	3.63 ± 0.39 ^d	2.19 ± 0.17 ^d	19.10 ± 1.70 ^a	19.69 ± 0.45 ^a	10.55 ± 0.97 ^c	13.01 ± 0.77 ^b	2.82 ± 0.21 ^d	2.39 ± 0.25 ^d
20	Ocimene	0.46 ± 0.11 ^{de}	1.87 ± 0.14 ^a	0.59 ± 0.08 ^d	nd	0.31 ± 0.09 ^e	nd	1.65 ± 0.15 ^b	0.90 ± 0.06 ^c
21	1,8-Cineole	1.66 ± 0.13 ^b	1.05 ± 0.20 ^{bc}	nd	2.16 ± 0.32 ^b	5.19 ± 1.83 ^a	nd	0.23 ± 0.03 ^c	0.27 ± 0.01 ^c
22	Gamma-Terpinene	0.43 ± 0.04 ^a	0.37 ± 0.04 ^b	0.15 ± 0.04 ^c	0.04 ± 0.00 ^d	0.13 ± 0.02 ^c	0.07 ± 0.02 ^d	0.04 ± 0.01 ^d	0.32 ± 0.04 ^b
23	Terpinolene	nd	nd	nd	nd	nd	nd	nd	0.05 ± 0.01
24	4-Ethyl- <i>m</i> -xylene	0.07 ± 0.00	nd	nd	nd	nd	nd	nd	nd
25	Beta-Caryophyllene	0.32 ± 0.02 ^a	0.06 ± 0.00 ^b	0.36 ± 0.05 ^a	nd	nd	nd	nd	nd
∑Esters		56.92	59.02	60.77	48.12	51.02	66.51	44.60	90.04
Ethyl alcohol		0.84	1.55	3.60	nd	nd	0.26	5.09	nd
∑Hydrocarbons		15.02	11.35	21.31	23.41	19.59	14.84	7.23	5
∑VOCs		72.78	71.92	85.68	71.53	70.61	81.61	56.92	95.04

Values (mean ± SD, $n = 3$) in the same line followed by a different letter are significantly different ($P < 0.05$). nd: not detected.



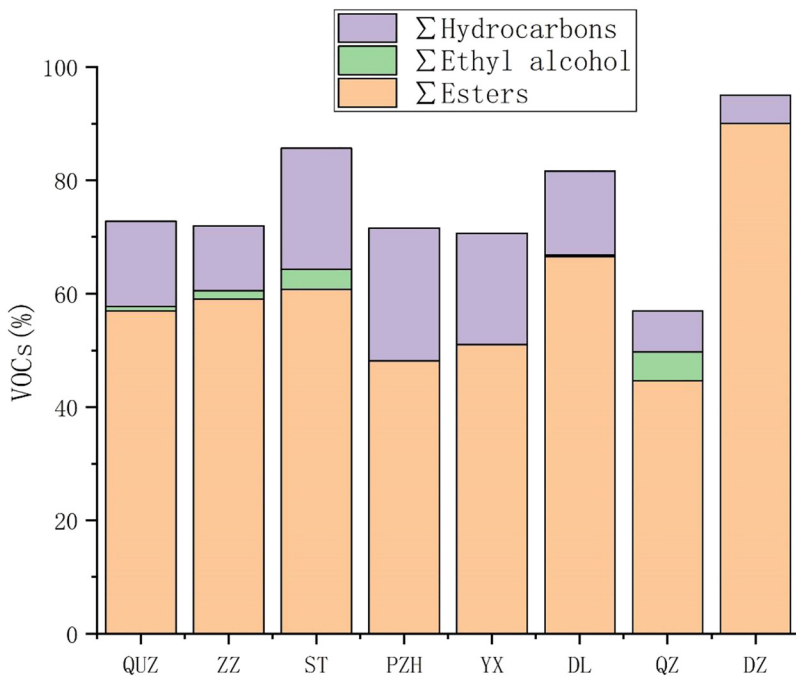


Fig. 3. Bar graph of HS-SPME/GC-MS analysis. VOCs: volatile organic compounds

The PCA and CA analysis results of the SPME/GC-MS were as follows. In Fig. 4A, the distributions of the first two principal components identified by the PCA are demonstrated, describing the cumulative 23.92% and 22.24% variance contributions, respectively. CA was used to describe the differences in the aroma profiles of PEL fruits based on the results of SPME/GC-MS analysis (Fig. 4B). When the Euclidean distance was 10, the PELs of ST, YX, DL, and QZ were assigned to the same group, which was similar to that of the PCA analysis, indicating that the fragrance signatures were similar.

The CA results and PCA plots of SPME/GC-MS were different from those of E-nose analysis, and the reason for this situation was the diverse analytical principles of E-nose and SPME/GC-MS (Li et al., 2017). Generally, the combination of SPME/GC-MS and E-nose can well evaluate the aroma profiles of the PEL fruits. These results could be the basis for further analysis of PEL origin.

3.6. Correlation analysis of origin parameters and constituents

Based on Pearson correlation coefficients, the correlation between geographic locations and the contents of PEL constituents was visualised using SPSS software, and a correlation coefficient of $|r| > 0.6$ was considered to indicate a moderate to high correlation (Dong et al., 2023). As shown in Fig. 5, east longitude negatively correlated with the fruit's brightness (b), K, Ca, and Mg, while had positive correlation with ethyl hexanoate and hexyl acetate. On the other hand, the



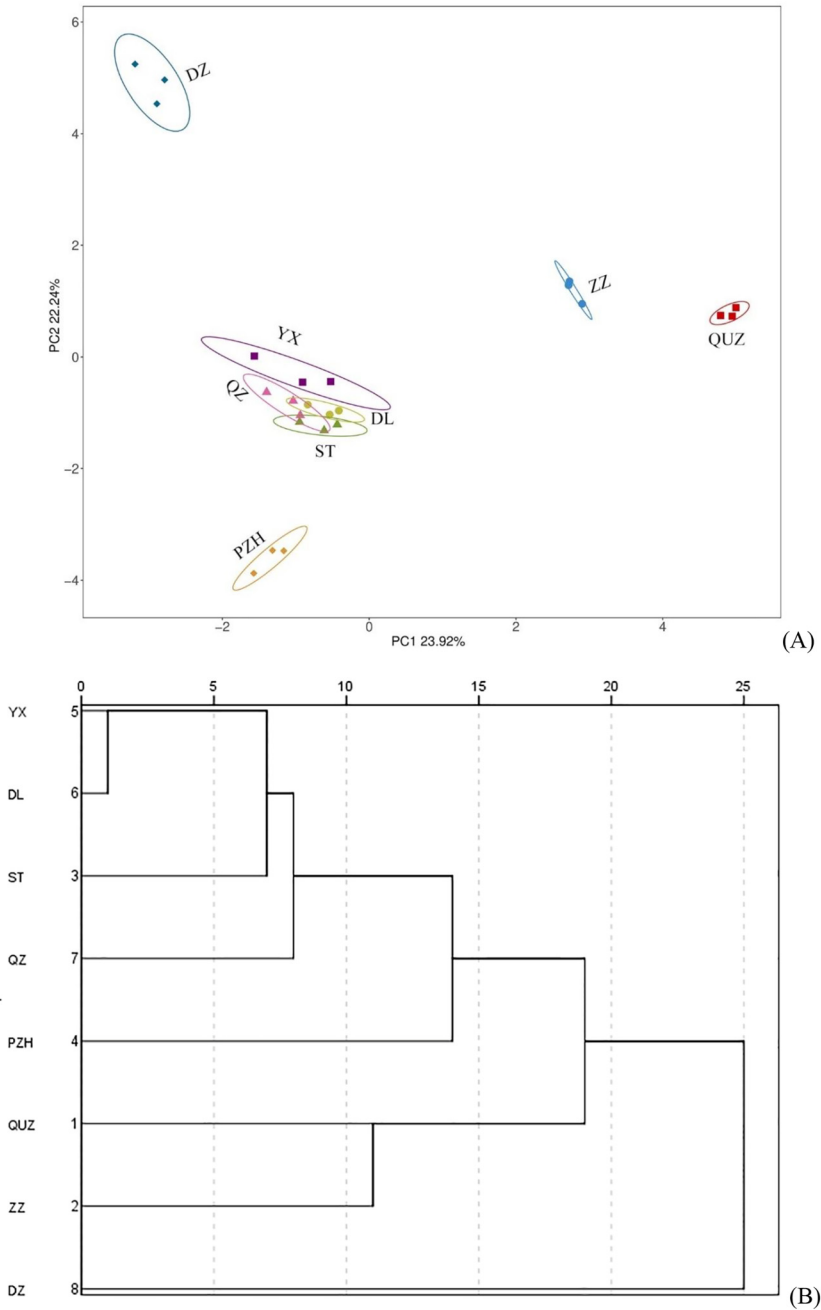


Fig. 4. Principal component analysis (A) and cluster analysis (B) of HS-SPME/GC-MS analysis



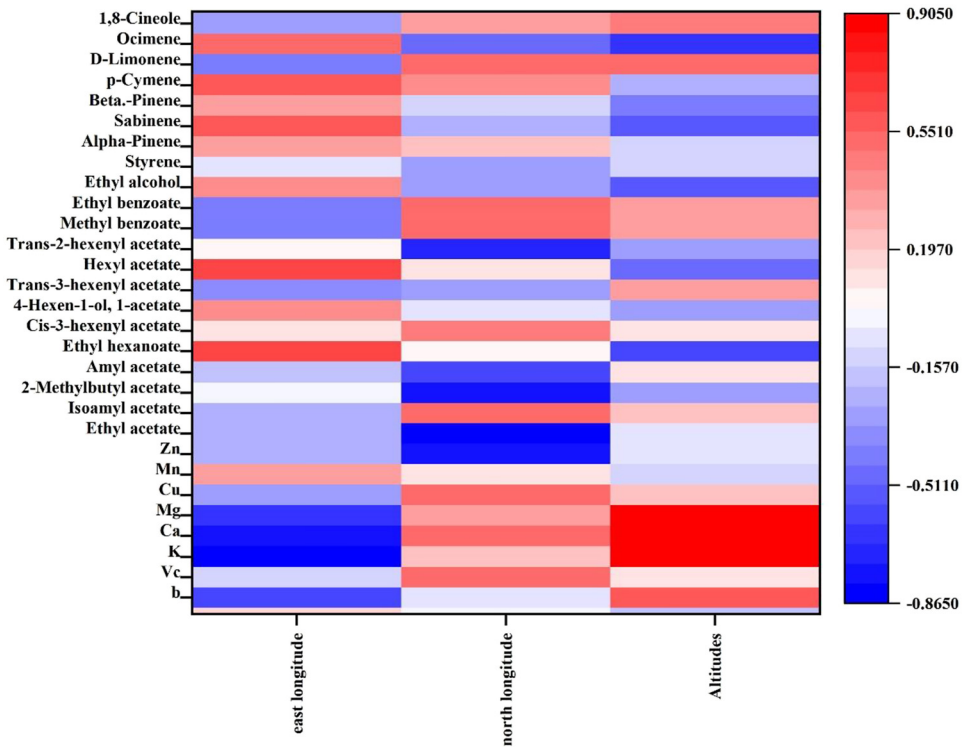


Fig. 5. Correlation analysis of origin parameters and constituents (Red is a positive correlation and blue is a negative correlation)

northern latitude displayed a negative correlation with Zn, ethyl acetate, 2-methylbutyl acetate, and trans-2-hexenyl acetate. Furthermore, the altitude demonstrated a positive correlation with K, Ca, and Mg.

4. CONCLUSIONS

The results of the present study showed that volatile compounds and conventional physico-chemical parameters in combination with chemometrics may differentiate the geographical origin of PEL. To the best of our knowledge, this is the first study on the differentiation of geographical origin of PEL based on colour parameters, Vc, mineral content, and volatile compounds, which is the novelty of the present work. The mineral content and volatile compounds of PELs were significantly different, which could be used to distinguish PEL from different habitats. Furthermore, present results clearly show the effectiveness of different parameter analyses on the characterisation of PEL from diverse origin. Finally, it should be noted that the data sets presented in the present study distinguish the sources of PEL, and may thus be used in PEL routine quality control and authentication efforts.



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