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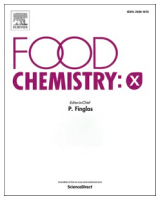

Comparative key aroma compounds and sensory correlations of aromatic coconut water varieties: Insights from GC × GC-O-TOF-MS, E-nose, and sensory analysis

Zizheng Li [1], Tao Wang [1], Hanwen Jiang, Wei-Ting Wang, Tao Lan, Lilan Xu, Yong-Huan Yun [*], Weimin Zhang

School of Food Science and Engineering, Key Laboratory of Tropical Fruits and Vegetables Quality and Safety for State Market Regulation, Hainan University, Haikou 570228, PR China

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Chemical compounds used in the study:
2-Acetyl-1-pyrroline (PubChem CID: 522834)
Acetoin (PubChem CID: 179)
2,3-Butanedione (PubChem CID: 650)
1-Nonanal (PubChem CID: 31289)
Octanal (PubChem CID: 454)
Isovaleraldehyde (PubChem CID: 11552)
Ethyl octanoate (PubChem CID: 7799)
Ethyl caproate (PubChem CID: 31265)
Ethyl acetate (PubChem CID: 8857)
1-heptanol (PubChem CID: 8129).

ABSTRACT

Aroma is a key criterion in evaluating aromatic coconut water. A comparison regarding key aroma compounds and sensory correlations was made between Thailand Aromatic Green Dwarf (THD) and Cocos nucifera L. cv. Wenye No. 4 coconut water using E-nose and GC × GC-O-TOF-MS combined with chemometrics. Twenty-one volatile components of coconut water were identified by GC × GC-O-TOF-MS, and 5 key aroma compounds were analyzed by relative odor activity value and aroma extract dilution analysis. Moreover, the combination of the E-nose with orthogonal partial least squares was highly effective in discriminating between the two coconut water samples and screened the key sensors responsible for this differentiation. Additionally, the correlation between volatile compounds and sensory properties was established using partial least squares. The key aroma compounds of coconut water exhibited positive correlations with the corresponding sensory properties.

1. Introduction

Coconut water, known as liquid endosperm, is a natural plant water formed by coconuts by storing nutrients in the form of liquid endosperm in coconuts (Yong et al., 2009). As a natural sports drink with a unique aroma and taste, tender coconut water can maintain a balance of the electrolyte concentration of human blood, which can help relieve summer heat and prevent dehydration. Moreover, it has been found to be effective against various health conditions, such as kidney stones and heart disease (Prado et al., 2015; Xu et al., 2022). Typically, Thailand Aromatic Green Dwarf (THD) is popular among consumers (Prades et al., 2012) and is known as the "Nam Hom" in Thailand. It is a variant of the dwarf coconut and is native mainly to Thailand's Tannen Sado district. Compared to ordinary coconuts, THD is smaller in size and features coconut water with a rich, creamy aroma and a distinctly sweet taste (Saensuk et al., 2016). Currently, its exceptional qualities have led to increasing popularity and have made it an important cash crop in Thailand. Furthermore, *Cocos nucifera* L. cv. Wenye No. 4, a recently developed aromatic coconut variety bred from THD and originating from Hainan, has bright coloration, delicate flesh, and sweet, aromatic water, making it particularly suitable for consumption as a fresh food.

Aroma is a key criterion in deciding the quality and marketing of coconut water. The unique aroma of coconut water is the product of a complex interplay of various aroma components. According to research, the volatile compounds found in aromatic coconut water have been classified into the following groups: ketones, alcohols, esters, aldehydes, lactones, terpenes, ethers, and heterocyclic compounds (De Marchi et al., 2015; Nasution et al., 2019; Shen et al., 2022; Zhang et al., 2023).

* Corresponding author.
E-mail address: yunyonghuan@hainanu.edu.cn (Y.-H. Yun).
[1] These authors contributed equally to this work.

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However, not all volatile components are detectable by human olfactory receptors, and therefore, these may have minimal impact on the overall aroma profile. Key aroma compounds with high odor intensity values and odor activity values (OAVs) significantly impact the aroma quality, for which they deserve much attention due to their massive research value (Feng et al., 2018). Moreover, the key aroma compounds in coconut water may vary slightly due to differences in coconut varieties, growing periods, and geographical origins. For instance, 2-acetyl-1-pyrroline (2-AP) was confirmed as the primary contributor to the creamy flavor of Nam-Hom, with the aroma described as "pandan-like" or "popcorn-like" (Luckanatinvong et al., 2018). As a natural aroma, 2-AP has also been found in aromatic rice and pumpkin leaves (Kiefl et al., 2013). However, the confirmation of 2-AP as the compound responsible for the distinctive aroma of Nam-Hom coconut water was not achieved through olfactometer analysis. In addition, Prades et al. identified 55 volatile components in THD by gas chromatography analysis and concluded that 2- and 3-methylbutan-1-ol and 1-hexanol significantly contributed to the aroma of coconut water (Prades et al., 2012). However, the existence of 2-AP was not detected in their analysis. Although there have been studies on 2-AP and the volatile components of coconut water, a systematic analysis to identify the key aromas of aromatic coconut water has not been conducted.

Molecular sensory science provides better approaches to identifying key aroma compounds by combining human senses with modern instruments, mainly based on instrumental analysis such as gas chromatography–mass spectrometry (GC–MS) and sensory analysis such as gas chromatography–olfactometry (GC–O), along with OAV and the aroma extract dilution analysis (AEDA) method (Amanpour et al., 2019; Gou et al., 2021; Regueiro et al., 2017; Song & Liu, 2018). Molecular sensory science aims to investigate the flavor system of food at the molecular level and to qualitatively, quantitatively, and descriptively analyze the aroma components of food (Gou et al., 2021). At present, molecular sensory science has been widely employed in the identification and characterization of key aroma compounds in various fruits, such as sweet orange, pineapple, pomegranate juice, and flat peach juice (Feng et al., 2018; George et al., 2023; Lu et al., 2023). Recently, two-dimensional comprehensive gas chromatography–olfactometry–time-of-flight mass spectrometry (GC × GC-O-TOF-MS) has gained widespread usage in the analysis of key aroma compounds in food products (Li et al., 2021; Li et al., 2023). Compared to GC-O-MS, GC × GC is equipped with two columns of different polarities in series, and the products separated in traditional one-dimensional gas chromatography are pulsed by a modulator to the second two-dimensional column with different properties for reseparation. It can switch between 1D and 2D analysis modes, which has the advantages of excellent resolution and fast analysis for complex food matrices, providing accurate results for the analysis of food flavors (Kiefl et al., 2013). Meanwhile, TOF–MS has strengths of high acquisition frequency, high sensitivity and selectivity. The combination of the two techniques effectively solves the issues of component coelution and the severe lack of peak capacity of traditional 1D GC. Moreover, the use of olfactometry in conjunction with two-dimensional gas chromatography enables the sniffing of aroma compounds under two-dimensional conditions. For instance, Zeng et al. identified 205 volatile components in Cordyceps militaris chicken soup by GC × GC-O-TOF-MS, which was 139 more than those detected by GC–MS (Zeng et al., 2020). Furthermore, 39 and 59 odor-active volatile components were detected by GC-O-MS and GC × GC-O-MS methods for the detection of aroma compounds in the leaves of moso bamboo, respectively (Shen et al., 2022). More aroma compounds (from fruits and herbs) were identified by GC × GC-O-MS than by GC-O-MS, which can be attributed to its high sensitivity and resolution. Meanwhile, an electronic nose (E-nose) is commonly employed to rapidly detect aroma components and analyze variations among different samples. It is an instrument that detects and collects gas composition and concentration through a series of chemical sensor arrays, similar to animal and human olfactory systems, and combines them with mathematical analysis methods for qualitative judgment and quantitative sample analysis (Shi et al., 2018). Typically, E-nose sensors exhibit nonspecificity and low selectivity, as well as strong stability and cross-selectivity for odorants or flavorants. The E-nose offers the advantages of simplicity, rapid analysis and functionality over traditional gas detection technologies. Despite these advantages, data from E-nose sensors may be more difficult to interpret because they cannot be easily correlated to any specific food substrate. Therefore, the integrated analysis of E-nose and GC–MS data is crucial for comprehensively analyzing aroma characteristics and volatile compounds. By analyzing the distinct metabolites of sea buckthorn wine and distilled liquor, the correlation between key volatile components and E-nose sensors was established (Xia et al., 2022). The results indicated that a positive correlation between seven sensors and alcohols and three sensors exhibited a positive correlation with acids, which demonstrated that the E-nose can differentiate sea buckthorn wine and distilled liquor based on their volatile components and detect trends in major aroma compounds rapidly. Currently, an increasing number of studies are employing the combination of GC–MS, GC × GC–MS and E-nose to comprehensively identify key compounds in food products (Wang et al., 2022).

To date, many instruments have been used for qualitative and quantitative analysis of volatiles, such as GC–MS and ion mobility spectrometry. However, few studies have used a combination of olfactory and GC × GC–TOF-MS to variously identify the key aroma compounds in coconut water (Gou et al., 2021). Thus, THD and Wenye No. 4 were selected as the research objects in this study. First, the aroma characteristics of the two types of coconut water were compared by E-nose combined with chemometrics. Then, the volatile components were detected by headspace solid-phase microextraction (HS-SPME) combined with GC × GC-O-TOF-MS based on molecular sensory science methods. Finally, a partial least squares (PLS) model was used to establish the relationship between key aromatic active compounds and sensory properties. This study aimed to identify the key aroma components of aromatic coconut water and evaluate the contribution of each component by using both the relative odor activity value (ROAV) and AEDA. Additionally, it further sought to compare the differences in aroma components and establish sensory correlations within aromatic coconut water varieties. Moreover, the identification of the key aroma compounds of aromatic coconut water will serve as a crucial basis for the high-quality development of aromatic coconut water.

2. Materials and methods

2.1. Samples and reagents

Sodium chloride (99.5 %), 2-methyl-3-heptanone (99 %), 1-heptanol (99.99 %), ethyl acetate (99.99 %), ethyl caproate (99.99 %), ethyl octanoate (99.5 %), isovaleraldehyde (99.99 %), octanal (99.99 %), 1-nonanal (99.99 %), 2,3-butanedione (99.99 %), acetoin (99.99 %), ethanol (99.99 %), 1-propanol (99.5 %) and acetaldehyde (99.99 %) were obtained from Macklin Biochemical Co. Ltd. 2-Acetyl-1-pyrroline (10 %w/w in Toluene) and *n*-alkane (C7-C40) were purchased from Sigma–Aldrich Chemical Co. (St. Louis, U.S.A.). Wenye No. 4 was an aromatic coconut with a maturity period of approximately 8 months harvested from the coconut germplasm repository of the Ministry of Agriculture and Rural Affairs in Wenchang, China. THD were harvested from the Thailand Aromatic Green Dwarf from Samut Sakhon Province, Thailand, with a ripeness of 7–8 months. Twenty coconuts of each variety were picked randomly at the planting site in January 2022. The coconuts were transported to the laboratory immediately after harvesting. Fresh coconut water was extracted, filtered and encapsulated in 50 mL centrifuge tubes immediately under sterile conditions. Packed samples were prefrozen at −20 ℃ for 24 h and then stored at −80 ℃ to maintain the original properties.

2.2. E-nose

E- nose (PEN 3 Airsense Analytics GmbH, Schwerin, Germany) was employed to analyze the aroma characterization of aromatic coconut water. Accurately 15 g of coconut water was loaded into a 40 mL headspace vial and equilibrated at 40 ℃ for 30 min to fill the vial with volatiles from the coconut water. The detection parameters of the electronic nose were as follows: the flow rate of the sample gas was 0.6 L/min; the sample preparation time was 5 s; the detection time was 200 s, and the cleaning time was 200 s to eliminate sample interference, reduce errors, and improve instrument sensitivity. Each sample was measured nine times. Table S1 presents the 10 sensors of the E-nose along with their corresponding sensitive substances.

2.3. Extraction of volatile components by HS-SPME

Accurately 15 g of coconut water and 0.15 g of NaCl were loaded into headspace vials (40 mL). Then, an internal standard of 0.5 μg 2-methyl-3-heptanone (0.816 μg/μl) diluted 1000 times was added into the headspace vial. The headspace vials were sealed and equilibrated at 40 ℃ for 20 mins. Volatile compounds were extracted from headspace vials by using an SPME fiber (50/30 μm, DVB/CAR/PDMS, Supelco, Bellefonte, PA, U.S.A.) at 40 ℃ for 40 mins. Before extraction, the GC inlet was used to pretreat the SPME fiber at 250 ℃ for 30 min, ensuring the elimination of any potential residues present in the fiber coating. After extraction, the fibers were transferred to the GC inlet and desorbed at 250 ℃ for 5 mins. The measurements of each sample were performed in triplicate.

2.4. Instrumentation and conditions of GC × GC-O-TOF-MS measurements

Aroma compounds of aromatic coconut water were detected by GC × GC-O-TOF-MS based on the method of Yang et al. with slight modifications (Yang et al., 2021). An Agilent 7890 gas chromatograph (Agilent Technology Co., Ltd, Santa Clara, CA, USA) equipped with an EI- TOFMS 0620 and an odor detector Sniffer 9100 (Brechbühler, Schlieren, Switzerland) was applied for the detection of volatile compounds. The GC × GC consisted of a DB-WAX column (60 m × 0.25 mm × 0.25 μm) and a DB-17 column (1.85 m × 0.18 mm × 0.18 μm). The initial temperature of the column was 40 ℃ for 5 mins, then raised to 230 ℃ at a rate of 4 ℃/min and kept for 2 mins. Ultrapure helium was used as the carrier gas, maintaining a constant flow of 1.0 mL min^{-1}. The ion source temperature was maintained at 200 °C, and the EI mass spectra were produced at 70 eV. The mass scan range was set to full scan mode at 33 *m/z*-350 *m/z* with a solvent delay of 6.3 mins. For the heating and cooling phases, a solid-state modulator SSM1800 (J&X Technologies, Shanghai, China) was placed between the two columns. The modulation period was set to 4 s, and the temperature in the cold zone was sustained at −51 ℃.

2.5. Qualification and quantitative analysis of volatile compounds

The qualitative analysis of volatile compounds in aromatic coconut water involved the comparison of mass spectrometry data, retention indices, and odors detected at the sniffer port. For key aroma compounds, the mass spectral library data, retention indices (RI) and odour descriptions of the sample extracts were compared with the standards. The MS data were analyzed by GC × GC-O-TOF-MS software (Agilent, CA, USA) and identified based on the NIST 14 mass spectrum database (https://www.nist.gov/srd/nist-special-database-14). The compound was identified initially when the degree of the match was greater than 800. The actual retention index (RI) of each compound was usually calculated by taking the retention time of its peak and *n*-alkanes (C7–C40) based on one-dimensional retention time using the following formula.

$$RI = 100N + 100n(t_{R_a} - t_{R_N})/(t_{R_{(N+n)}} - t_{R_N}) \quad (1)$$

where *N* denotes the carbon number of the lower alkane, and n is the difference in carbon number between the two *n*-alkanes that surround the compound. The variables t_{R_a}, t_{R_N}, and $t_{R_{(N+n)}}$ denote the retention times of the unknown compound, lower alkane, and upper alkane, respectively.

The odor characteristics of the volatile compounds were analyzed by a professional sensory evaluator and then compared to the aroma descriptions of volatile compounds on the Professional Aroma Compounds website (https://thegoodscentscompany.com/).

Semiquantitative analysis of volatile compounds in coconut water samples was carried out by the normalization method based on the peak area of the internal standard compound (2-methyl-3-heptanone) and the peak area of the compound.

2.6. Relative odor activity value (ROAV)

ROAV is defined as the ratio of the OAV of an aroma compound to that of the compound with the highest aroma contribution in a sample. It is commonly used to assess the impact of an aroma component on the overall aroma profile. Compounds exhibiting a ROAV value of ≥1 can be identified as key aroma compounds that significantly contribute to the overall aroma profile of coconut water. In contrast, aroma compounds with a ROAV value less than 1 have a moderate effect on the overall aroma. The ROAV is calculated as follows.

$$ROAVi \approx 100 \times \frac{Ci}{Ti} \times \frac{T\max}{C\max} \quad (2)$$

where $ROAV_i$ is the relative odor activity value of a volatile component; C_i and C_{max} are the relative contents of a volatile component and the volatile component contributing the most to the odor, respectively; T_i is the odor threshold of a volatile component; and T_{max} is the odor threshold of the volatile component with the highest odor contribution. The odor thresholds for the volatile compound refer to the book *Odor thresholds* (Gemert, 2003).

2.7. Aroma extract dilution analysis (AEDA)

The key aroma compounds of coconut water were identified by AEDA. Accurately 2 μL of coconut water dilutions were analyzed by GC × GC-O-TOF-MS and rated with a three-point intensity scale (1 = weak, 2 = medium, 3 = strong) for the perceived intensity at the sniffing port. The compounds were sequentially diluted with 2n (n = 0, 1, 2, 3, 4, 5…. …..) by varying the splitting ratio of the GC inlet. The flavor dilution multiples (FD factors) were obtained after each dilution, which were 1, 2, 4, 8, 16, 32, 64, 128, 256, and 512.

2.8. Qualitative descriptive analysis (QDA)

Sensory analysis was performed in a sensory room (20 ± 1) ℃ by 12 already standardized and trained panelists (5 males and 7 females). Before sensory analysis, all panel members underwent training focused on coconut water and standard aroma compounds to achieve their ability to identify, describe, and distinguish between various aroma characteristics. The evaluation team members initially proposed the aroma terms for coconut water, and then the terms were discussed and initially screened, and irrelevant terms were removed. The aroma terms for this study were determined to be popcorn, creamy, sweet, grassy, sour, and woody. Reference compounds for aroma are as follows: popcorn flavor (10 μg/ml of 2-acetyl-1-pyrroline solution), sweet (honey), grassy (1 μg/ml of *cis*-3-hexenol in glycerol triacetate), sour (1 mg/ml of acetic acid solution), and woody flavor (5 g of oak wood chips in 100 mL of 10 % ethanol–water solution). A 10-point intensity scale (0 = none, 1 = very low, 9 = very high) was used for each sensory term for

three repeated assessments. The final sensory score was determined by calculating the average score of the terms.

2.9. Statistical analysis and software

The radar chart and histograms were plotted using Origin 2023 (Origin Lab Corporation, Northampton, MA, USA). Differences between sample groups were analyzed by analysis of variance (ANOVA) with $P < 0.05$ indicating significant differences between volatile components, and Duncan's multiple-range test was performed by using SPSS 26 software (IBM, Armonk, NY, USA). Orthogonal partial least squares–discriminant analysis (OPLS–DA) is analyzed on the web page https://www.metaboanalyst.ca/.

3. Results and discussion

3.1. Analysis of coconut water volatile components based on E-nose

The E-nose was employed to rapidly assess the aroma characteristics of coconut water, which is widely applied for aroma identification and differentiation. The use of the E-nose helped to avoid the subjectivity of sensory evaluation by simulating human sniffing to obtain overall aroma characteristics about the sample (Baietto & Wilson, 2015; Wu et al., 2021). Slight variances in volatile compounds can be recognized by differences in sensor response values. The radar chart can visualize the intensity and differences in volatile components between THD and Wenye No. 4. As shown in Fig. 1A and Table S2, the radar charts of the two types of coconut water had similar shapes, indicating that the response of the volatiles to the E-nose sensor was highly similar in THD and Wenye No. 4. The response value of the E-nose sensor is highly correlated with the content of the corresponding volatile components of coconut water. Sensors S2, S8, S6, S7, and S1 were more sensitive and had higher response values for volatile components of the two types of coconut water. This indicated that the volatile components of the two types of coconut water had high and different contents of alcohols, methyl substances, and aromatic compounds, which had a significant impact on the aroma of THD and Wenye No. 4. Meanwhile, the response values of the S10, S9, S5, S4, and S3 sensors were low and showed only slight differences, suggesting that the alkane, aromatic composition, hydrogen, and ammonia levels in the coconut water were not significantly changed after selective breeding and local domestication.

Among the 10 sensors of the E-nose, the response values of THD and Wenye No. 4 were significantly different ($P < 0.01$) in the remaining sensors, except for the S4 sensor. The response values of Wenye No. 4 were higher than THD for each sensor, with higher response values of 4.65, 4.23, and 3.80 for S8, S6, and S2 sensors, respectively, which indicates that alcohols, methyl substances, and nitrogen oxides were higher than THD for Wenye No. 4.

A comprehensive analysis of the volatile components of coconut water cannot be performed by a single radar chart of the sensor. Therefore, OPLS–DA was employed for the volatile components of the two types of coconut water in this study. As presented in Fig. 1B, a clear

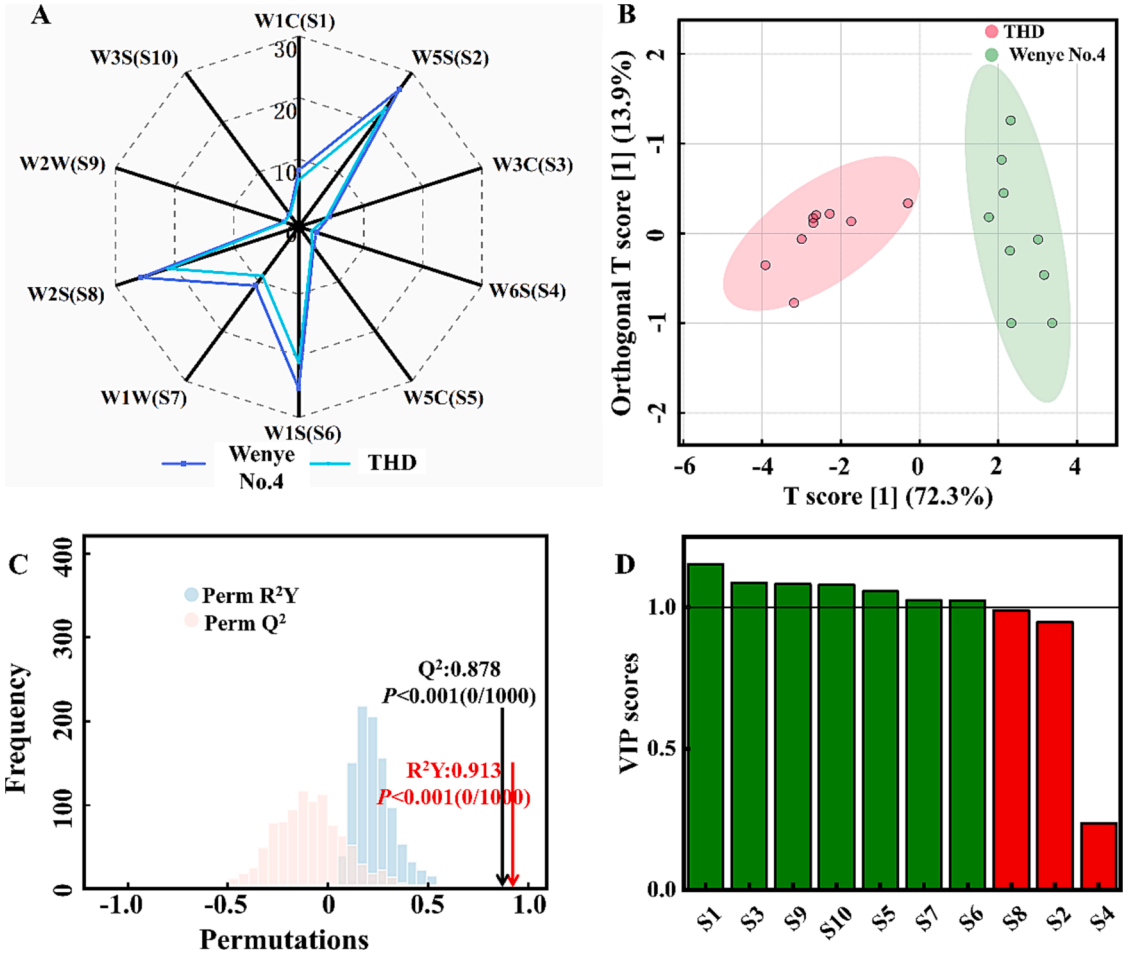

Fig. 1. Radar chart and orthogonal partial least squares discriminant analysis (OPLS–DA) analysis of coconut water; (A) Radar plot of the electronic nose of Thailand Aromatic Green Dwarf (THD) and Wenye No. 4; (B) OPLS–DA score plot of E-nose response values for coconut water; (C) Result map of 1000 cross-validations of the OPLS–DA model (0/1000 indicates that 0 permutations out of 1,000 permutation tests are better than the current model.); (D) Variable importance in projection (VIP) plot.

distinction between Wenye No. 4 and THD was observed, with THD located in the first and fourth quadrants, while Wenye No. 4 was distributed in the second and third quadrants. This suggests that there were significant differences in the aroma composition of coconut water from different varieties. Notably, R^2X is the model fit to X, R^2Y is the model fit to Y and Q^2 is the model predictive ability. The model is considered optimal if the model parameters R^2Y and Q^2 are between 0.5 and 1. The model had a good explanation rate and predictability in this study, with an R^2X of 0.862, R^2Y of 0.912, and Q^2 of 0.878. The OPLS–DA model was cross-validated with 1000 permutation tests to prevent overfitting, and the *P* values of Q^2 and R^2Y were less than 0.05. The results showed that the *P* values of Q^2 and R^2Y were less than 0.001, suggesting that the model has good robustness (Fig. 1C) (An et al., 2022). Meanwhile, to assess the degree of contribution of sensors to the distinction of coconut water samples, a variable importance in projection (VIP) plot of OPLS–DA was also generated. The VIP value could filter the variables of variance that had important contributions to the model classification, and the variables with VIP values greater than 1 were generally considered the main variance variables (Tang et al., 2022). As depicted in Fig. 1D, the VIP values of the S1, S3, S9, S10, S5, S7 and S6 sensors were greater than 1, which indicated that the S1, S3, S9, S10, S5, S7 and S6 sensors contributed significantly to the sample classification. Thus, these sensors were available as specific sensors to distinguish between the two types of coconut water. Based on the above analysis, the two types of coconut water can be effectively divided by the combination of E-nose and OPLS–DA, and it also indicated that there existed significant differences in the aroma composition of THD and Wenye No. 4. Therefore, this study further explored the aroma characteristics and differences between the two types of coconut water at the molecular level using GC × GC-O-TOF-MS.

3.2. Identification of volatile components of coconut water by GC × GC-O-TOF-MS

The volatile components of THD and Wenye No. 4 were separated and characterized by GC × GC-O-TOF-MS (Fig. S1) and identified by mass spectrometry, RI values and olfactory detection. A total of 21 volatile components were detected, as shown in Table 1, including 7 alcohols, 6 esters, 4 aldehydes, 3 ketones, and 1 furan compound. The furan was detected in this study, which is rare in coconut water volatiles. These compounds generated specific aroma characteristics, such as roasted grains, creaminess, fruity, and grassy flavors, which together constitute the distinct aroma profile of coconut water (Nasution et al., 2019). In addition, there were 11 volatile components common to two types of coconut water, namely, ethanol, 1-propanol, 2-methyl-1-propanol, 1-hexanol, 1-octanol, ethyl acetate, ethyl caproate, methyl octanoate, ethyl octanoate, nonanal, and acetoin. It can be seen from Fig. 2A that there were certain similarities and differences between THD and Wenye No. 4 in aroma composition. Furthermore, alcohols, as important aroma components of coconut water, were higher in Wenye No. 4 than in THD, which was consistent with the results of E-nose analysis in the GC × GC-TOF-MS detection.

Table 1
Identification of volatile compounds in two types of coconut water by GC × GC–TOF–MS.

No.	Formula	Compound	RI	Content/μg/kg		Qualitative Method	Odor description
				THD	Wenye No.4		
Alcohols							
1	C_2H_5OH	Ethanol	924	28.83 ± 0.69[a]	35.28 ± 2.2[b]	MS/RI/O	strong alcoholic, ethereal medical
2	C_3H_8O	1-Propanol	1032	0.13 ± 0.01[a]	0.15 ± 0.01[a]	MS/RI/O	alcoholic fermented, musty
3	$C_4H_{10}O$	2-Methyl-1-propanol	1091	0.03 ± 0[a]	–	MS/RI	ethereal, winey, cortex
4	$C_4H_{10}O$	1-Butanol	1142	0.28 ± 0.02[a]	0.23 ± 0.01[b]	MS/RI	fusel oil, sweet, balsam, whiskey
5	$C_6H_{14}O$	1-Hexanol	1349	0.17 ± 0.01[a]	0.11 ± 0.01[b]	MS/RI	ethereal, fusel oil, fruity, sweet, green
6	$C_7H_{16}O$	1-Heptanol	1452	0.18 ± 0.01[a]	–	MS/RI	violet herbal, green, sweet, woody, peony
7	$C_8H_{18}O$	1-Octanol	1554	0.43 ± 0.02[a]	0.11 ± 0.01[b]	MS/RI	waxy, green, orange, aldehydic, rose, mushroom
			Subtotal	30.05	35.88		
Esters							
8	$C_4H_8O_2$	Ethyl acetate	868	2.36 ± 0.11[a]	3.01 ± 0.13[b]	MS/RI/O	ethereal, fruity, sweet, weedy, green
9	$C_7H_{14}O_2$	Methyl caproate	1184	–	0.07 ± 0[a]	MS/RI	fruity, pineapple, ether
10	$C_8H_{16}O_2$	Ethyl caproate	1232	0.15 ± 0.01[a]	0.08 ± 0.00[b]	MS/RI	sweet, fruity, waxy, green
11	$C_9H_{18}O_2$	Methyl octanoate	1390	0.04 ± 0[a]	0.01 ± 0[b]	MS/RI	waxy, green, sweet, orange, aldehydic, vegetable, herbal
12	$C_{10}H_{20}O_2$	Ethyl octanoate	1434	0.83 ± 0.05[a]	0.09 ± 0.01[b]	MS/RI	Fruity, wine, waxy, sweet, brandy, pear
13	$C_{12}H_{24}O_2$	Ethyl caprate	1638	0.04 ± 0	–	MS/RI	sweet, waxy, fruity, oily, brandy
			Subtotal	3.42	3.26		
Aldehydes							
14	C_2H_4O	Acetaldehyde	744	0.13 ± 0.01[a]	–	MS/RI/O	pungent, ethereal, aldehydic, fruity
15	$C_5H_{10}O$	Isovaleraldehyde	905	0.14 ± 0.01[a]	–	MS/RI	ethereal, aldehydic, chocolate, peach, fatty
16	$C_8H_{16}O$	Octanal	1289	0.07 ± 0.01[a]	–	MS/RI	aldehydic, waxy, citrus, orange, peel, green, fatty
17	$C_9H_{18}O$	1-Nonanal	1395	0.19 ± 0.09[a]	0.08 ± 0.01[a]	MS/RI/O	waxy, aldehydic, rose, fresh, orange, peel, fatty
			Subtotal	0.53	0.08		
Ketones							
18	$C_4H_6O_2$	2,3-Butanedione	965	0.35 ± 0.01[a]	–	MS/RI/O	strong butter, sweet, creamy, pungent, caramel
19	$C_4H_8O_2$	Acetoin	1288	1.09 ± 0.04[a]	0.23 ± 0.01[b]	MS/RI/O	sweet, buttery, creamy, dairy, milky, fatty
20	C_6H_9NO	2-Acetyl-1-pyrroline	1345	0.09 ± 0[a]	–	MS/RI/O	popcorn, toasted, grain, malty
			Subtotal	1.53	0.23		
Furans							
21	C_5H_6O	2-Methylfuran	878	0.5 ± 0.03[a]	–	MS/RI	ethereal, acetone, chocolate
			Subtotal	0.5	–		

"-" indicates that the compound was not detected.
[a, b, c] means within a row with different superscripts significantly differ ($P < 0.05$), n = 3.
Different identification methods, including mass spectrometry (MS), retention indices (RI), odor description (O).

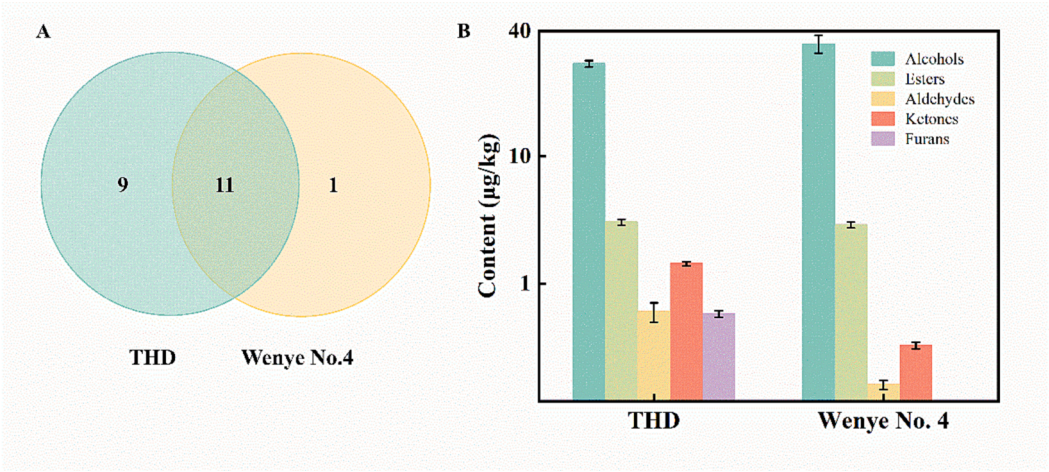

Fig. 2. Comparison of volatile components of the two coconut water types. (A) Venn diagram of the volatile components of coconut water. (B) The volatile components of the two coconut water types.

Alcohols had the highest content of THD and Wenye No. 4 volatiles, and these volatiles can provide coconut water with aromatic characteristics such as sweet, green, fruity, wine and ether. Meanwhile, alcohols, which are organic compounds characterized by the presence of a hydroxyl (–OH) functional group, can exhibit diverse odors depending on their chemical structure. In coexistence with aldehydes and esters in coconut water, they can provide coconut water with floral and fresh fruit aroma (Nasution et al., 2019). In particular, ethanol had the highest content of 28.83 μg/kg and 35.28 μg/kg, respectively, and these values exceeded the sum of other volatile components. Esters contributed fruity and waxy aroma to coconut water, and ethyl acetate was the most prominent of these and was verified as a key aroma compound in wines (Niu et al., 2017; Wang et al., 2021). Xu et al. analyzed the volatile components of coconut water using GC–MS and believed that esters played a predominant role in the overall aroma of coconut water (Xu et al., 2022). Then, ketones were found to be a significant component of the aroma profile of coconut water, with acetoin exhibiting the highest concentration among them. The presence of acetoin was found in both green and yellow coconut water, contributing to buttery and creamy flavor (da Fonseca et al., 2009). In addition, acetoin exists in a variety of foods, such as palm toddy, cheeses, and Chinese steamed breads, and is considered to contribute significantly to their aroma (Chen et al., 2022; Huang et al., 2023; Lasekan & Abbas, 2010). Aldehydes, which are products of lipid oxidation, were also detected at low levels in THD and Wenye No. 4 and could provide aroma characteristics of grassy, fruity and fatty to coconut water.

It can be clearly seen from Fig. 2B that there were marked differences in both the types and contents of volatile compounds of the two types of coconut water. In total, 20 volatile components were detected in THD (Table S3), comprising 7 alcohols (83.40 %), 5 esters (9.49 %), 4 aldehydes (1.47 %), 2 ketones (4.25 %), and 1 furan compound (1.39 %). Compared to the most recent study on “Nam Hom” coconut water, volatile components were commonly detected, including ethyl acetate, 1-butanol, ethyl caproate, 2-AP, 1-hexanol, methyl octanoate, ethyl octanoate, 1-heptanol, and 1-octanol (Luckanatinvong et al., 2018). A previous study identified 24 volatile components in “Nam Hom” coconut water, and the quantities detected were generally consistent with those found in our study. In contrast, acids were not found in this study, which might be due to their high polarity or low content in the complex matrix of coconut water, making it difficult to separate and detect them effectively on the DB-WAX column. A total of 12 volatile components in Wenye No. 4 were detected (Table S4), including 5 alcohols (90.95 %), 5 esters (8.26 %), 1 aldehyde (0.20 %), and 1 ketone (0.58 %). To compare the differences between the volatile components of THD and Wenye No. 4, a significance analysis was performed. ANOVA indicated that there was no significant difference observed between 1-propanol and 1-nonanal in the two types of coconut water ($P > 0.05$), and significant differences existed for all other volatiles ($P < 0.05$). In regard to the overall quantity of detected volatile components, Wenye No. 4 was higher than THD. However, it was primarily ethanol that played a decisive role in this difference in content. Apart from ethanol, THD had a greater variety and concentration of volatile components compared to Wenye No. 4. The results above showed that the aroma quality of the aromatic coconut changed to a certain extent after local selection and domestication, which may be attributed to the different geographical locations, growth periods and climatic environments of the coconut.

3.3. *Characterization of key aroma compounds by ROAV*

To verify the key aroma compounds of coconut water, ROAV was applied to assess the contribution of volatile components to aroma. A higher ROAV value indicated a stronger impact of a compound on the aroma of coconut water (Sun et al., 2022). ROAV offered an advantage over OAV values by considering the contribution of odor compounds to the overall aroma rather than assessing each compound’s contribution individually. This allowed for further identification of the main components of the aroma and provided more practical odor assessment results (Su et al., 2022; Wang et al., 2023). In total, 10 key aroma compounds of 21 volatile compounds in two types of coconut water were identified by the ROAV, including 1 alcohol, 3 esters, 3 aldehydes and 3 ketones (Table 2). Four key aroma compounds were commonly detected in THD and Wenye No. 4, namely, ethyl acetate, ethyl caproate, 1-nonanal, and acetoin.

Based on the data presented in Table 2, 10 key aroma compounds were identified among the 20 volatile components of THD, in descending order of contribution: 2,3-butanedione (strong butter, sweet, creamy, pungent, caramel), 2-AP (popcorn, toasted, grain, malty), ethyl acetate (ethereal, fruity, sweet, weedy, green), ethyl caproate (sweet, waxy, fruity, oily, brandy), isovaleraldehyde (ether flavor, chocolate flavor, peach flavor, fat flavor), acetoin (sweet, buttery, creamy, dairy, milky, fatty), 1-nonanal (Waxy, aldehydic, rose, fresh, orange, peel, fatty), octanal (pungent, ethereal, aldehydic, fruity), ethyl octanoate (fruity, wine, waxy, sweet, brandy, pear), and 1-heptanol (violet herbal, green, sweet, woody, peony). Ketones were found to be the primary aroma-contributing compounds in THD. In particular, 2,3-butanedione had the highest ROAV value despite its low content, and this substance was associated with the creamy flavor of coconut water. It is worth noting that the ethanol with the highest content was not identified as a key aroma compound because of its high threshold value. Meanwhile, 4 components of Wenye No. 4 were identified: ethyl acetate, ethyl

Table 2
Identification of key aroma compounds in two kinds of coconut water by ROAV.

No.	Species	Compound	Odor detection threshold (μg/kg)	ROAV		Qualitative Method
				THD	Wenye No.4	
1	Alcohols	1-heptanol	5.4	1.67	–	MS/RI/STD
2	Esters	Ethyl acetate	5	24.05	100	MS/RI/O/STD
3		Ethyl caproate	1	7.53	14.05	MS/RI/STD
4		Ethyl octanoate	19.3	2.21	–	MS/RI/STD
5	Aldehydes	Isovaleraldehyde	1.2	5.92	–	MS/RI/STD
6		Octanal	0.8	4.29	–	MS/RI/STD
7		1-Nonanal	1.1	8.8	12.69	MS/RI/O/STD
8	Ketones	2,3-Butanedione	0.18	100	–	MS/RI/O/STD
9		Acetoin	14	3.96	2.78	MS/RI/O/STD
10		2-Acetyl-1-pyrroline	0.12	35.56	–	MS/RI/O/STD

Different identification methods, including mass spectrometry (MS), retention indices (RI), odor description (O), and standard compounds (STD).

octanoate, 1-nonanal, and acetoin. Notably, 1-nonanal was ranked third in the aroma contribution, but at the same level as ethyl caproate, owing to the slightly smaller threshold of ethyl caproate compared to 1-nonanal. Comparing the key aroma compounds of the two types of coconut water by ROAV, it was found that THD has a greater variety and amount of key aroma compounds than Wenye No. 4. All of the aroma compounds present in Wenye No. 4 were also found in THD, suggesting that Wenye No. 4 retained some of its aroma components during the selection and domestication process, while others were lost.

3.4. Characterization of key aroma compounds by AEDA

While ROAV is useful for assessing the contribution of key aroma compounds to the overall aroma of coconut water, it does not fully reflect the perception of these compounds by human olfaction due to differences in threshold data. Hence, the volatile components of THD and Wenye No. 4 were filtered by AEDA in this study to eliminate the shortcomings in ROAV. The level of contribution of each volatile compound to the aroma is determined by the FD factor in AEDA. Specifically, there was a positive correlation between the FD factor and the contribution of key aroma compounds to the overall aroma (Liu et al., 2018). In general, volatile compounds with an FD factor value of 16 or higher are considered key aroma compounds in food products. However, the standard is not absolute. For food products with a light aroma such as coconut water, using an FD factor value of 16 may not be sufficient to fully reflect its key aroma compounds, and thus, the standard FD value must be adjusted. Determining the components with an FD factor value of 2 or higher as key aroma compounds allowed for a more comprehensive assessment of the aroma characteristics of coconut water. As revealed in Table 3, AEDA analysis revealed the presence of 8 aroma compounds in aromatic coconut water, including 2 alcohols, 1 ester, 2 aldehydes, and 3 ketones. In particular, the FD values of 7 key aroma compounds ranged from 2 to 512. Ethanol, 1-propanol, ethyl acetate, 1-nonanal, and acetoin could be smelled in the two types of coconut water, and there was no significant difference in FD values, thus indicating that these were not the main reasons for the difference between THD and Wenye No. 4.

A total of 7 key aroma compounds were verified in THD, among which 2-AP was found to be the most influential in terms of the overall aroma, despite its low content of 0.09 μg/kg. This compound presented the strongest odor intensity, as indicated by its high FD value of 512. In previous studies, the variation in the content of 2-AP corresponded well with the change in the aroma and sweetness of coconut water and may be the main reason for the formation of aromatic coconut aroma (Luckanatinvong et al., 2018). The existence of 2-AP was detected in a variety of aromatic coconut species, and the synthesis of this compound was found to be associated with a genotype of CnAMADH2 (De Marchi et al., 2015; Dumhai et al., 2019; Saensuk et al., 2016). Remarkably, the odor intensity of 2,3-butanedione was intermediate, while acetoin and ethyl acetate had the same FD value as 2,3-butanedione but exhibited a weak odor intensity. The other 6 compounds with FD $\leq$ 4 were perceived with a weak intensity, and they still made a distinct contribution to the overall aroma characteristics of aromatic coconut water. Meanwhile, in Wenye No. 4, the analysis revealed the presence of 5 key aroma compounds, among which ethyl acetate and ethanol exhibited the highest FD values, ethyl acetate possessed a medium odor intensity, and the other 4 compounds were sniffed with a weak intensity. Moreover, although the FD value of ethyl acetate in both coconut water samples was 8, its odor intensity was observed to be higher in Wenye No. 4 than in THD. This could be attributed to the higher content of ethyl acetate in Wenye No. 4, as well as differences in sensory thresholds due to the presence of different substrates containing the same aroma compounds (Plutowska & Wardencki, 2008). Based on the above analysis, in actual sniffing, more key aroma compounds and higher odor intensity were observed in THD, which is basically consistent with the ROAV results.

3.5. Comparative analysis of key aroma compounds characterized by ROAV and AEDA

A Venn diagram was constructed based on the key aroma compounds detected in coconut water (Fig. S2). Five compounds were detected as

Table 3
Identification of key aroma compounds in two types of coconut water by AEDA.

No.4	Compound	Odor	FD factor		Odor intensity		Qualitative Method
			THD	Wenye No.4	THD	Wenye No.4	
1	Ethanol	strong alcoholic, ethereal medical	4	8	Weak	Weak	MS/RI/O/STD
2	1-Propanol	alcoholic, fermented, fusel, musty	2	2	Weak	Weak	MS/RI/O/STD
3	Ethyl acetate	ethereal, fruity, sweet, weedy, green	8	8	Weak	Medium	MS/RI/O/STD
4	Acetaldehyde	pungent, ethereal, aldehydic, fruity	1	–	Weak		MS/RI/O/STD
5	1-Nonanal	waxy, aldehydic, rose, fresh orris, orange, peel	2	2	Weak	Weak	MS/RI/O/STD
6	2,3-Butanedione	strong butter, sweet, creamy, pungent, caramel	8	–	Medium		MS/RI/O/STD
7	Acetoin	sweet, buttery, creamy, dairy, milky, fatty	8	4	Weak	Weak	MS/RI/O/STD
8	2-Acetyl-1-pyrroline	popcorn, toasted, grain, malty	512	–	Strong		MS/RI/O/STD

Different identification methods, including mass spectrometry (MS), retention indices (RI), odor description (O), and standard compounds (STD).

key aroma compounds for THD by both methods, including 2-AP, 2,3-butanedione, ethyl acetate, acetoin, and 1-nonanal. On the other hand, ethyl acetate, 1-nonanal, and acetoin were verified as key aroma compounds in both methods for Wenye No. 4. Ethyl acetate and acetoin were identified as the key aroma compounds in THD and Wenye No. 4 by both methods, suggesting that these were the key aroma substances commonly existing in coconut water. In both methods, 2,3-butanedione and 2-AP were identified as significant contributors to the aroma of THD, and ethyl acetate was identified as the compound with the highest aroma contribution to Wenye No. 4 in both methods. Based on the analysis above, it can be concluded that there is a certain consistency between AEDA and ROAV. Nevertheless, there was variability observed in the magnitude of the contribution of each compound to the aroma of coconut water obtained by both methods. For instance, AEDA analysis revealed that 2-AP in THD was found to have a strong odor intensity, but it ranked second in the degree of aroma contribution determined by ROAV. Similarly, 2,3-butanedione was considered to be the most critical compound responsible for the aroma of THD in ROAV, while the odor intensity was rated as medium by olfactometry. Although ethyl caproate was listed second by ROAV in Wenye No. 4, it was not smelled by the sensory evaluator through AEDA. Whereas acetoin and 1-nonanal were smelled in the AEDA method, they were ranked after ethyl caproate in the ROAV method. These variabilities may be related to the fact that the threshold values used in the ROAV method were from the literature and have a large variability with the actual situation of this experiment.

Particularly, it is based on thresholds to evaluate the extent of aroma contribution in both ROAV and AEDA methods. Instrumental analysis is utilized in ROAV, which allows for a rapid determination of characteristic aroma components. However, it should be noted that the method does not take into account the impact of the matrix on the volatility and threshold of the aroma compounds. AEDA is a method that combines instrumental analysis with sensory analysis, thereby providing more accurate and reliable results. However, AEDA relies on the subjective evaluation of aroma by professional sensory evaluators, which makes it susceptible to personal biases and may introduce some level of subjectivity. In summary, it is a limitation of relying on one method to determine the key aroma compounds of coconut water, and no analytical method can perform a comprehensive analysis of the key aroma compounds of the samples. Hence, validation and supplementation from multiple methods are essential for accurate results.

Consequently, based on the compounds that contributed more to the overall aroma of coconut water in both methods, five key aroma compounds of THD were verified as 2-AP, 2,3-butanedione, ethyl acetate, acetoin, and 1-nonanal, and 3 key aromas of Wenye No. 4 were identified, namely, ethyl acetate, 1-nonanal, and acetoin.

3.6. Sensory evaluation

QDA was utilized to analyze the aroma profiles of the aromatic coconuts. The evaluation team employed six sensory terms: popcorn, creamy, sweet, grassy, sour, and woody. Based on the data presented in Fig. 3A, THD exhibited significantly higher levels of popcorn, creamy, and sweet aromas compared to Wenye No. 4, indicating the dominance of these three aroma characteristics in the aroma of THD. This distinction can be attributed to the presence of 2-AP and 2,3-butanedione. While Wenye No. 4 scored slightly higher in terms of sour and grassy aromas compared to THD, the difference was not statistically significant ($P < 0.05$). Overall, there were substantial differences in the aromatic profiles of the two aromatic coconuts. THD displayed prominent notes of popcorn, creamy, and sweet, which could be a key factor contributing to

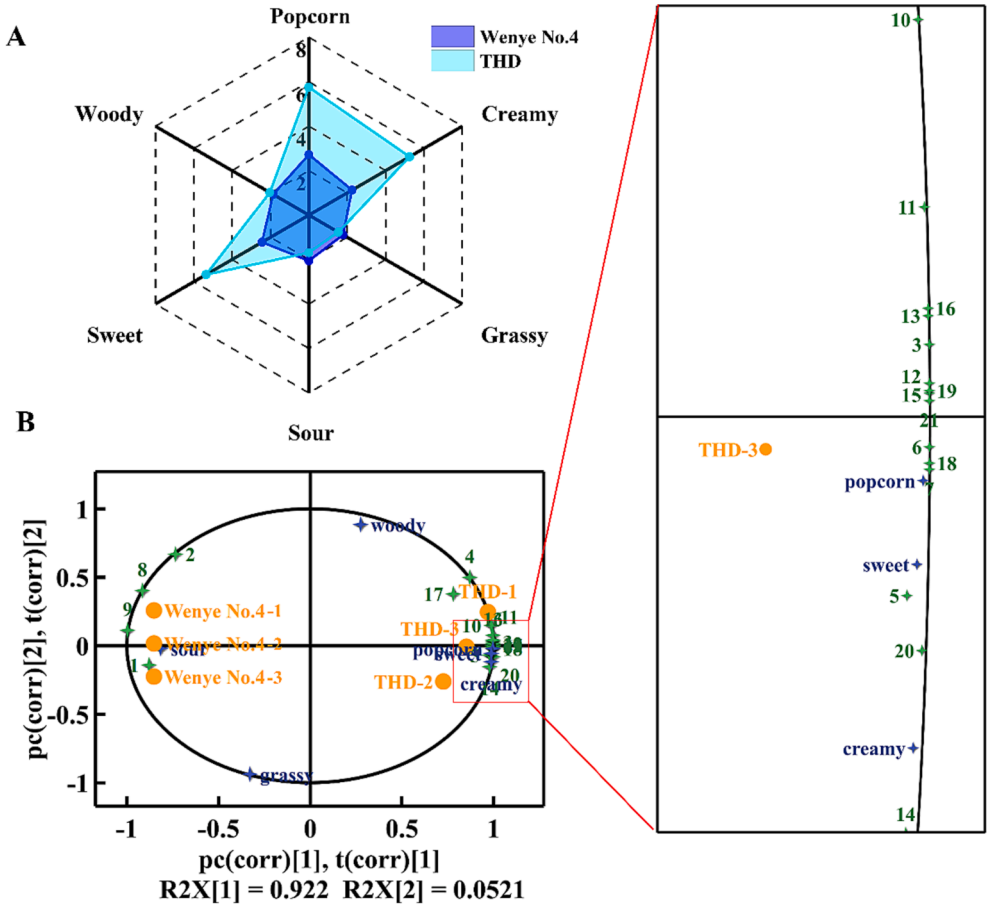

Fig. 3. Sensory analysis (A) and correlation between sensory properties and aroma compounds of coconut water established by the PLS model (B).

its popularity among consumers.

Additionally, PLS can establish the correlation between sensory scores and volatile compounds to explore the intricate relationship between aroma compounds and sensory properties of THD and Wenye No. 4. The quantitative results of 21 aroma compounds in the two samples were analyzed using the PLS model, as shown in Fig. 3B. The R^2 value represents the explanatory ability of the model, while Q^2 reflects its predictive ability. The PLS model demonstrated excellent performance, with R^2 and Q^2 values of 0.974 and 0.726, respectively. These values affirm its accuracy in representing the true information within the samples. From Fig. 3B, it was evident that "grassy" and "sour" contributed to distinguishing THD from Wenye No. 4, although the correlation with Wenye No. 4 was weak, possibly due to its relatively low sensory score. Furthermore, 1-propanol, ethyl acetate, methyl hexanoate, and ethanol exhibited a significant positive correlation with the sour. Notably, ethyl acetate displayed a stronger correlation with sour compared to grassy. This occurrence may arise from the interaction of ethyl acetate with other compounds or sample matrices, such as 1-butanol, 1-octanol, and ethyl hexanoate, independent of its behavior within the food matrix or flavor blend. The remaining four sensory properties, namely, popcorn, creamy, sweet, and woody, were identified as the main sensory characteristics of THD. Additionally, 1-octanol, 2-AP, 2,3-butanedione, 1-heptanol, acetoin, isovaleraldehyde, ethyl caproate, ethyl octanoate, and octanal exhibited significant positive correlations with these sensory properties.

4. Conclusion

The key aroma compounds of THD and Wenye No. 4 and the contribution level were investigated by E-nose and GC × GC-O-TOF-MS. The results demonstrated that the E-nose combined with chemometrics is an effective tool for classifying different types of coconut water, and OPLS–DA revealed that sensors S1, S3, S9, S10, S5, S7 and S6 played a crucial role in distinguishing between the two types of coconut water. A total of 21 volatile components, including 7 alcohols, 6 esters, 4 aldehydes, 3 ketones, and 1 furan compound, were detected by GC × GC-O-TOF-MS. ROAV and AEDA effectively highlighted the pronounced differences in the key aroma compounds between the two coconut water types. Five key aroma compounds, including 2-AP, 2,3-butanedione, ethyl acetate, acetoin, and 1-nonanal, were identified as key aroma compounds of THD. Furthermore, ethyl acetate, 1-nonanal, and acetoin were confirmed as the key aroma compounds in Wenye No. 4 coconut water. From a sensory analysis perspective, THD and Wenye No. 4 exhibited aroma profiles predominantly characterized by aromas such as popcorn, creamy, sweet, grassy, sour, and woody. The pivotal aroma compounds in THD, including 2-AP, 2,3-butanedione, and acetoin, displayed positive correlations with popcorn, creamy, and sweet flavors. This study has revealed the key aroma compounds of coconut water and enhanced the comprehension of its aroma. Furthermore, the complementarity of the E-nose and GC × GC-O-TOF-MS developed technical support for in-depth research on the aroma characteristics of coconut water.

CRediT authorship contribution statement

Zizheng Li: Writing – original draft, Methodology, Data curation. **Tao Wang:** Writing – review & editing, Investigation. **Hanwen Jiang:** Writing – review & editing, Investigation. **Wei-Ting Wang:** Writing – review & editing. **Tao Lan:** Writing – review & editing, Investigation. **Lilan Xu:** Writing – review & editing. **Yong-Huan Yun:** Writing – review & editing, Project administration, Funding acquisition, Conceptualization. **Weimin Zhang:** Resources, Project administration.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.fochx.2024.101141.

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