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Chemical Profiling and Sensory Analysis Reveal Quality Differentiation in Baimudan White Tea Processed from Three Major Fujian Tea Cultivars

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Abstract

White tea quality is primarily determined by its chemical composition, which varies significantly among cultivars. This study aimed to elucidate the chemical basis underlying quality differentiation in Baimudan white tea produced from three major Fujian tea cultivars: "Zhenghe Dabaicha" (ZHDB), "Fuan Dabaicha" (FADB), and "Fuding Dahaocha" (FDDH). Headspace solid-phase microextraction coupled with gas chromatography–mass spectrometry (HS-SPME-GC-MS), liquid chromatography–mass spectrometry (LC-MS), and quantitative descriptive analysis (QDA) were employed to characterize volatile compounds, amino acids, and saccharides. Odor Activity Values (OAVs) and Taste Activity Values (TAVs) were calculated to identify key contributors to sensory perception. Results showed that theanine, glutamic acid, asparagine, and serine were the primary contributors to umami taste, especially in ZHDB and FADB. Sweetness differences were largely due to sucrose, serine, and asparagine. OAV analysis further identified 22 critical aroma compounds: methyl salicylate, linalool, and β-ionone predominantly imparted floral notes, while β-ocimene, benzaldehyde, and geraniol enhanced sweet and fruity aromas. In contrast, (*Z*)-3-hexenol, (*Z*)-3-hexenal, and (*E*)-2-hexenal contributed grassy and refreshing characteristics, together defining the unique aroma profiles of each cultivar. This study provides an integrated chemical and sensory framework for understanding white tea quality variation, offering a theoretical basis for targeted flavor modulation.

Keywords: white tea; volatiles; amino acids; sensory profile

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1. Introduction

Fujian white tea, renowned for its delicate flavor and health-promoting properties, plays a pivotal role in China's tea industry [1]. Globally, white tea production is primarily concentrated in China, with Fujian province being the leading region, notably Fuding and Zhenghe. While it represents a niche segment compared to green or black tea, China's

white tea output has experienced significant growth, reaching approximately 93,800 tons, accounting for 2.6% of the total tea yield in 2024 [2]. Moreover, extensive cellular (in vitro) and animal (in vivo) studies have further indicated white tea's potential anti-cancer, anti-diabetic, and anti-inflammatory activities [3]. High-quality white tea typically presents a refreshing, sweet, and mellow taste, accompanied by fresh floral and downy (silvery-white hair) aromas [4,5]. Its production process is comparatively simple, requiring only withering and drying of fresh leaves to complete primary processing [3]. Consequently, cultivar-dependent differences in endogenous metabolites of fresh leaves can strongly influence the sensory quality of the final tea, even under identical processing conditions.

In recent years, considerable progress has been made in the study of white tea germplasm resources and flavor characteristics. Systematic quality evaluations and biochemical analyses have confirmed that varietal traits play a decisive role in shaping flavor profiles. For instance, statistical analyses comparing Zhenghe Caicha tea with four mainstream white tea varieties from major production regions demonstrated notable quality differences. White tea produced from Caicha contained abundant volatile alcohols, terpenes, ketones, aldehydes, and esters, resulting in a unique floral and fruity aroma [6]. Similarly, Jinggu white tea from Yunnan exhibited stronger fruity and sweet notes than both Fujian and other Yunnan cultivars, a difference primarily driven by key volatiles such as linalool and benzeneacetaldehyde, underscoring the influence of cultivar origin on sensory properties and its implications for targeted quality control [7]. Xiaobai white tea, derived from local Fujian population varieties, was reported to contain higher levels of amino acids, polyphenols, and volatile substances such as Damascus ketone and cedarwood alcohol, which together enhanced its sweetness, taste, and floral aroma [8]. The albino cultivar "Ming guan", originating from "Bai jiguan", displayed a favorable amino acid-to-phenol ratio that evolved during withering. Key metabolites, including geraniol and (*E*)-2-hexenal, contributed to fruity and floral characteristics, positioning this cultivar as a promising germplasm for premium white tea products [9]. Furthermore, studies on Oolong tea cultivar-derived white teas have shown that varieties such as Zimeigui exhibit superior taste and aroma, attributed to higher concentrations of linalool, geranyl formate, and epigallocatechin gallate. Distinctive volatile components including trans-2-nonenal and methyl salicylate also imparted darker liquor colors, richer floral, and cultivar-specific aromas, and a slightly astringent taste, distinguishing them from traditional white tea varieties [10].

Baimudan white tea, also known as white peony, is a premium category of white tea produced from tender buds and young leaves [11]. The cultivars "Zhenghe Dabaicha" (ZHDB), "Fuan Dabaicha" (FADB), and "Fuding Dahaocha" (FDDH), all native to Fujian Province, are widely regarded as the most suitable for white tea production and represent the predominant varieties used in its manufacture [12]. Baimudan teas derived from these cultivars are valued for their refined floral aroma and mellow taste, leading to their widespread cultivation across China. However, despite their popularity, they exhibit distinct quality characteristics in actual production, and the biochemical basis underlying this sensory diversity remains insufficiently characterized.

Systematic and comparative investigations of Baimudan white tea from Fujian's three principal cultivars–Zhenghe Dabaicha (ZHDB), Fuan Dabaicha (FADB), and Fuding Dahaocha (FDDH)–are currently scarce, despite extensive evidence that cultivar traits exert a decisive influence on the sensory quality of white tea. This gap limits understanding of how cultivar-specific metabolite profiles determine the sensory characteristics of high-grade white tea and constrain strategies for targeted breeding and quality control. The present study aims to elucidate the extent to which differences in volatile compounds, amino acids, and sugars among these cultivars account for variations in floral aroma, freshness, and

umami intensity. It is hypothesized that each cultivar exhibits a distinct metabolite composition that underlies its characteristic sensory profile, and that these compositional differences can be quantitatively linked to specific aroma–taste attributes. To test this hypothesis, the present study applies Headspace Solid-Phase Microextraction Gas Chromatography–Mass Spectrometry (HS-SPME-GC-MS), 6-aminoquinolyl-n-hydroxysuccinyl carbamate (AQC) derivative liquid chromatography–tandem triple-quadrupole mass spectrometry (AQC-LC-QQQ-MS), and Gas Chromatography–Mass Spectrometry (GC-MS) to investigate differences in volatile compounds, amino acids, and sugar profiles among these cultivars. By integrating these results with quantitative descriptive analysis (QDA), we identified differential metabolites and clarified their contributions to key sensory attributes such as floral aroma, freshness, and umami intensity in Baimudan white tea. This integrative approach not only deepens mechanistic insights into the formation of signature flavor profiles but also establishes a theoretical foundation for optimizing the selection and utilization of cultivars in white tea production.

2. Materials and Methods

2.1. Experimental Materials

Fresh tea leaves of *Camellia sinensis cv.* 'Zhenghedabaicha' (ZHDB), *Camellia sinensis cv.* Fuandabaicha (FADB), and *Camellia sinensis cv.* Fudingdahaocha (FDDH) were collected in spring 2024 from the Tea Germplasm Resource Garden of Wuyi University (118.00° E, 27.71° N) for Baimudan white tea production. The picking standard was uniformly set as one bud with one or two leaves. To ensure consistency among varieties, 25 kg of fresh leaves from each cultivar were evenly spread on adjacent bamboo sieves at a uniform thickness for withering. White tea processing parameters were adapted from established protocols with modifications to optimize tea quality [13]. Withering was performed in an indoor chamber at ~26 °C with semi-ventilation, no supplemental lighting, and relative humidity maintained at 60–70% for 49 h, followed by oven drying at 70 °C for 1 h. All subsequent analyses were conducted on three independent biological replicates.

Chemicals used included methanol, acetonitrile, n-hexane, and isopropanol (all HPLC grade), methoxyamine hydrochloride (99%), and pyridine (99%) purchased from Merck KGaA (Darmstadt, Germany). N,O-Bis(trimethylsilyl)trifluoroacetamide (99%), trimethylchlorosilane (99%), deuterated 3-hexanone (HPLC grade), C8–C40 n-alkane mix, and sodium chloride (analytical grade) were obtained from Shanghai Aladdin Biochemical Technology Co., Ltd (Shanghai, China). The AccQ·Fluor™ amino acid derivatization kit was sourced from Waters Corporation (Milford, MA, USA), while 32 carbohydrate reference standards (HPLC grade) were procured from Shanghai ANPEL Scientific Instrument Co., Ltd. (Shanghai, China).

Instrumentation included a GX-5888 tea roaster (Quanzhou Gaoxiang Machinery Trading Co., Ltd., Quanzhou, China), Agilent 7890B-7000C GC-MS system (Agilent Technologies, Santa Clara, CA, USA), Sciex 4500 QTrap triple quadrupole mass spectrometer (Sciex, Framingham, MA, USA), Shimadzu Nexera X2 LC-30A HPLC system (Shimadzu Corporation, Kyoto, Japan), IKA MS3 basic vortex mixer (Shanghai Pengqi Scientific Instruments Co., Ltd., Shanghai, China), KQ-100E ultrasonic cleaner (Kunshan Ultrasonic Instruments Co., Ltd., Kunshan, China), Heraeus Multifuge X3R refrigerated centrifuge (Thermo Fisher Scientific, Waltham, MA, USA), XD-DCY-24Y nitrogen evaporator (Shanghai Xida Instrument Co., Ltd., Shanghai, China), and a CentriVap freeze dryer (Shanghai Hechen Technology Co., Ltd., Shanghai, China).

2.2. Sensory Evaluation and Quantitative Descriptive Analysis

Quantitative descriptive analysis (QDA) was conducted following the method of Zheng et al., with slight modifications [14–16]. A sensory evaluation panel was formed by recruiting university students and teachers holding a Level 3 (senior) tea-tasting certification. Panelists were selected according to the Chinese National Standard GB/T 16291.1-2012 Sensory analysis—General guidance for the selection, training and monitoring of assessors—Part 1: Selected assessors [17]. The initial screening involved aroma recognition tests and descriptive ability assessments. Ultimately, seven trained panelists (three males and four females, aged 22–35 years) were selected. All had a minimum of two years' experience in sensory evaluation of tea.

Panel training and performance evaluation were conducted in three phases. In Phase 1, the panelists evaluated three representative white tea samples prepared according to GB/T 23776-2018 Methodology for sensory evaluation of tea to generate a preliminary list of descriptors [18]. Through focus group discussions and reference to literature, consensus was reached on nine sensory attributes: five aroma descriptors (fresh, floral, fruity, sweet, tip) and four taste descriptors (umami, sweetness, mellowness, bitterness). In Phase 2, QDA was applied to evaluate all white tea samples. For each evaluation, 3.0 g of dry tea was placed into a 150 mL cylindrical porcelain cup, infused with 150 mL of freshly boiling water (100 °C), and brewed for 5 min before the infusion was filtered. The serving order of samples was randomized across panelists following a balanced incomplete block design to minimize carryover effects. Each sample was evaluated in duplicate across two separate sessions.

Aroma attributes were identified and quantified using the quantitative descriptive analysis (QDA) method. Five key aroma descriptors were used: fresh—light grassy note with faint cucumber freshness; floral—subtle orchid fragrance; fruity—apple-like aroma; sweet—honey-like and sweet–fat notes; tip—distinctive, delicate "hao xiang" (bud aroma) characteristic of white tea. Panelists scored each attribute on a five-point intensity scale (0 = not perceived; 3 = moderate; 5 = strong). Between samples, panelists rinsed their mouths with purified water at room temperature. All sessions were conducted in the morning (09:00–11:00) to avoid sensory fatigue.

2.3. Aroma Compound Analysis

Volatile compounds were analyzed using headspace solid-phase microextraction coupled with gas chromatography–mass spectrometry (HS-SPME-GC-MS), with parameters optimized based on validated protocols [19]. Powdered tea samples (500 mg, liquid nitrogen ground) were placed in 20 mL headspace vials with saturated NaCl solution and 10 µL deuterated 3-hexanone internal standard (50 µg/mL). After equilibration at 60 °C for 5 min, volatiles were extracted with a 120 µm DVB/CAR/PDMS fiber for 15 min and desorbed at 250 °C for 5 min. GC-MS employed a DP-5 MS capillary column (30 m × 0.25 mm × 0.25 µm) with helium (>99.99%) at 1.2 mL/min. The oven program started at 40 °C for 3.5 min, increased to 100 °C at 10 °C/min, to 180 °C at 7 °C/min, and then to 280 °C at 25 °C/min with a 5 min hold. Electron ionization (70 eV) was operated in selected ion monitoring mode. Compounds were identified using the NIST 2020 library and retention indices validated with C8–C40 n-alkanes. Quantification was performed by internal standard calibration with peak area ratios. A full list of detected volatile compounds is provided in Supplementary Table S1.

2.4. Amino Acid Profiling

Amino acids were quantified following previously described methods [20]. Ground tea samples (0.2 g) were vortexed with 40 mL ultrapure water, sonicated for 30 min at 45 kHz,

and centrifuged for 5 min. The supernatant (10.0 μL, filtered through a 0.22 μm membrane) was mixed with 70.0 μL AccQ-Fluor borate buffer (pH 8.8) and 20.0 μL AccQ-Fluor reagent, then incubated at 55 °C for 10 min before LC-MS analysis. Separation was carried out on a Waters HSS T3 C18 column (1.8 μm, 2.1 mm × 150 mm) at 40 °C using mobile phase A (10 mmol/L ammonium formate, pH 6.0) and B (acetonitrile) at 0.3 mL/min. Gradient elution proceeded from 0% to 20% B in 12 min, to 35% B in 16 min, to 90% B in 18 min, and returned to 5% B in 20 min. MS conditions were set to electrospray ionization (ESI, 4500 V) in positive MRM mode, with auxiliary gas at 0.38 MPa and a temperature of 550 °C.

2.5. Carbohydrate Profiling

Targeted quantification of 32 plant-derived carbohydrates was conducted using gas chromatography–mass spectrometry (GC-MS). Freeze-dried white tea samples (20 mg) were homogenized by ball milling (30 Hz, 1.5 min), extracted with 500 μL methanol:isopropanol (3:3:2, $v/v/v$), vortexed for 3 min, and sonicated at 4 °C for 30 min. After centrifugation (12,000 rpm, 3 min), 12.5 μL of the supernatant was combined with 20 μL of internal standard solution (250 μg/mL), concentrated under nitrogen, and subsequently lyophilized. Derivatization was carried out by sequentially adding 100 μL methoxyamine hydrochloride (15 mg/mL) at 37 °C for 2 h, followed by 100 μL BSTFA for 30 min at 37 °C. The derivatized solution was diluted with 800 μL n-hexane, filtered through a 0.22 μm membrane, and transferred into amber vials for GC-MS analysis.

Chromatographic separation employed a DB-5MS capillary column (30 m × 0.25 mm × 0.25 μm) with helium as the carrier gas at 1 mL/min and a split ratio of 5:1. The oven program started at 160 °C for 1 min, increased to 200 °C at 6 °C/min, then to 270 °C at 10 °C/min, and finally to 320 °C at 20 °C/min, holding for 5.5 min. MS parameters were set as follows: transfer line at 280 °C, electron ionization (70 eV), ion source at 230 °C, quadrupole at 150 °C, and selected ion monitoring (SIM) mode with a 1 μL injection volume and 4 min solvent delay. Quantification was achieved using external calibration curves constructed by plotting analyte concentration ratios (x-axis) against peak area ratios (y-axis). Carbohydrate contents in samples were determined by substituting measured peak area ratios into the linear equations of the corresponding standard curves.

2.6. Calculation of Taste Active Value (TAV) and Odor Activity Value (OAV)

Taste active value (TAV) and odor activity value (OAV) were applied to evaluate the relative contributions of taste- and aroma-active compounds in white tea [21,22]. A TAV ≥ 1 indicated that the compound concentration reached or exceeded its taste perception threshold, contributing directly and significantly to the flavor profile, whereas a TAV < 1 implied weak or negligible taste impact. Similarly, an OAV ≥ 1 denoted that the compound concentration surpassed its olfactory detection threshold, resulting in a perceptible aroma contribution, while an OAV < 1 suggested little or no olfactory influence.

$$\mathrm{TAV} = \frac{C}{T} \tag{1}$$

where (C) represents the concentration (mg/g) of a taste compound, and (T) denotes its taste perception threshold. The Taste Activity Value (TAV) is used to assess the contribution of a taste compound to the overall flavor profile.

$$\mathrm{OAV} = \frac{C1}{T1} \tag{2}$$

where ($C1$) represents the concentration (mg/g) of an aroma compound, and ($T1$) denotes its odor perception threshold. The Odor Activity Value (OAV) is used to evaluate the relative importance of aroma compounds in the overall aroma profile.

2.7. Statistical Analysis

Experimental data were organized using Excel 2007 (Microsoft). Statistical analyses and data visualization were performed using GraphPad Prism 8 (version 8.0.1, GraphPad Software) and TBtools (version 2.210) [23]. Data are expressed as mean ± standard deviation (SD) of three independent biological replicates. For each measured parameter (aroma compounds, amino acids, carbohydrates), a one-way analysis of variance (ANOVA) was conducted to assess differences among the three tea cultivars. When ANOVA results were significant ($p < 0.05$), Duncan's multiple range test (DMRT) was used for post-hoc multiple comparisons. Duncan's test was selected because it is well established in food chemistry and agricultural product quality assessment, providing higher statistical power than more conservative methods

3. Results

3.1. Sensory Quality Analysis of Baimudan White Tea Processed from Fujian's Primary Cultivars

The sensory panel employed in this study was the same as that used in our previous work [16], in which panel performance was validated using PanelCheck software (Version.1.4.2) and found to meet the acceptable criteria for sensory evaluation of tea. In the present study, each sample was evaluated twice in independent sessions by the same trained panelists, and no significant differences ($p > 0.05$) were found between replicate evaluations, indicating good repeatability and consistent scoring. Therefore, the sensory data presented below are based on a validated and reliable panel.

The sensory evaluation results of Baimudan produced from the three major Fujian cultivars are summarized in Supplementary Table S2. All samples achieved total sensory scores above 90, confirming their suitability for further analysis. ZHDB displayed plump silver buds with a grayish-green appearance, while FADB presented connected buds and leaves with a gray-green tone. Liquor color assessments indicated that ZHDB and FDDH had bright (clear and vibrant) apricot-yellow infusions, whereas FADB showed a slightly deeper yellow. The infused leaves of ZHDB appeared plump and bright, FADB leaves were soft and bright, and FDDH leaves were tender and uniformly bright.

Sensory profiling revealed distinct aroma and taste characteristics among the three teas. ZHDB was marked by pronounced floral notes, FADB by mild floral notes with a green apple nuance, and FDDH by a prominent downy aroma. In terms of taste, FADB was more robust, while FDDH was slightly sweeter. Quantitative descriptive analysis (Figure 1b) evaluated five aroma attributes (fresh, floral, tip, fruity, sweet) and four taste attributes (umami, sweetness, mellowness, bitterness). ZHDB and FADB exhibited similar profiles, both scoring significantly higher for fresh, floral, and umami attributes than FDDH. In contrast, FDDH scored significantly higher in downy aroma and sweetness.

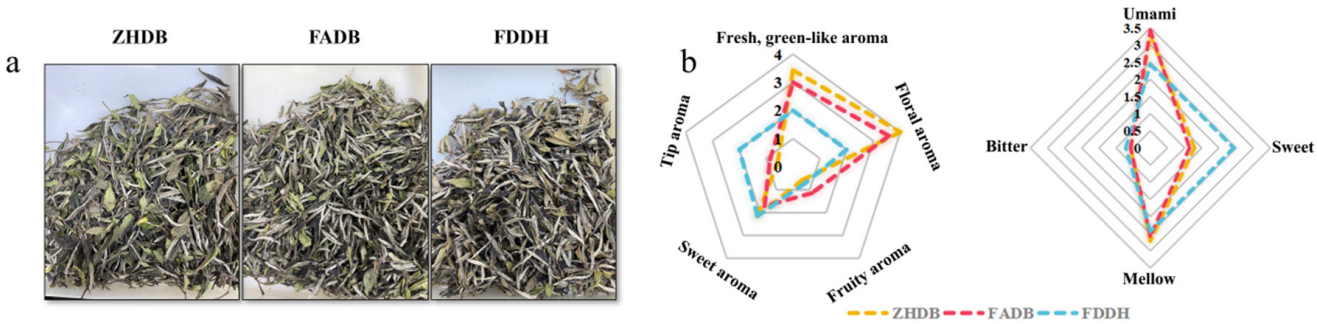

Figure 1. Quantitative Descriptive Analysis of Baimudan white teas from ZHDB, FADB, FDDH cultivars. (**a**): Dried Baimudan tea samples from ZHDB, FADB, and FDDH cultivars; (**b**): Radar chart of Quantitative Descriptive Analysis (QDA).

3.2. Amino Acid Profiling of Baimudan White Tea Processed from Fujian's Primary Cultivars

Amino acid analysis identified 21 detectable amino acids across ZHDB, FADB, and FDDH samples (Figure 2a). LC-MS results indicated that theanine (Thea), asparagine (Asn), and glutamine (Gln) were the most abundant. ZHDB and FADB exhibited similar amino acid accumulation patterns, while FDDH differed markedly in levels of serine (Ser), proline (Pro), valine (Val), leucine (Leu), isoleucine (Ile), aspartic acid (Asp), methionine (Met), tyrosine (Tyr), tryptophan (Trp), Asn, and Gln compared with ZHDB and FADB ($p < 0.05$). No significant differences were detected between ZHDB and FADB. These disparities may explain the distinct taste characteristics observed among cultivars. To evaluate the contribution of amino acids to taste, taste activity values (TAVs) were calculated based on reported thresholds [24,25]. The four umami-related amino acids consistently exhibited higher TAVs in ZHDB and FADB compared with FDDH, whereas FDDH showed higher TAVs for the sweet-tasting amino acids Asn and Ser. In addition, statistical correlation analysis was performed to quantitatively link amino acid composition with sensory attributes (Supplementary Table S3). Pearson correlation coefficients revealed that the concentrations of umami-related amino acids, including Thea, GABA, Asp, and glutamic Glu, were strongly and positively correlated with the sensory umami intensity ($R > 0.90$, $p < 0.05$). Similarly, sweet-tasting amino acids such as Ser and Asn exhibited strong positive correlations with perceived sweetness scores ($R > 0.90$, $p < 0.05$). Overall, these results provide quantitative evidence supporting the role of specific amino acids in shaping the characteristic flavor profiles of the different cultivars.

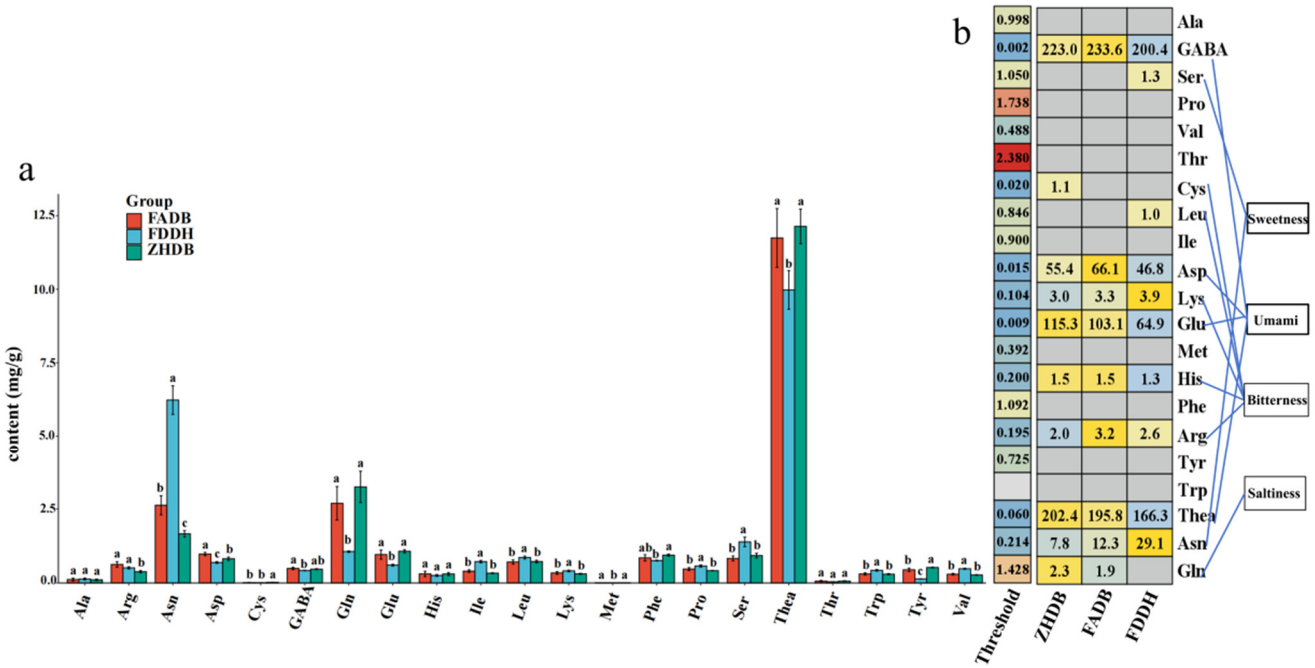

Figure 2. Amino acid composition analysis of Baimudan white teas from ZHDB, FADB, and FDDH. (**a**): Bar plot showing the contents of individual amino acids. Duncan's test was used to compare whether there were significant differences between the means of two groups. Different letters indicate significant differences among group means at $p < 0.05$. Abbreviations: Ala, alanine; GABA, γ-aminobutyric acid; Ser, serine; Pro, proline; Val, valine; Thr, threonine; Cys, cysteine; Leu, leucine; Ile, isoleucine; Asp, aspartic acid; Lys, lysine; Glu, glutamic acid; Met, methionine; His, histidine; Phe, phenylalanine; Arg, arginine; Tyr, tyrosine; Trp, tryptophan. (**b**): Heatmap of threshold values and TAV (Threshold Aroma Value) for amino acid components. Numerical values represent calculated TAVs, with gray boxes indicating TAV < 1. Connecting lines represent flavor attributes of amino acids with TAV > 1.

These compositional differences likely underlie the stronger umami perception in ZHDB/FADB and the greater sweetness in FDDH.

3.3. Carbohydrate Profiling of Baimudan White Tea Processed from Fujian's Primary Cultivars

Carbohydrates, as key metabolites, contribute to structural support, energy storage, and sensory perception. Quantitative analysis revealed 19 monosaccharides (Figure 3a) and 6 polysaccharides (Figure 3b) across ZHDB, FADB, and FDDH, with sucrose, glucose, fructose, and myo-inositol being the most abundant. Significant variation in carbohydrate distribution was observed among cultivars. FDDH contained significantly higher levels of myo-inositol compared with ZHDB and FADB ($p < 0.05$), while sucrose levels were significantly higher in ZHDB (2.97 ± 0.20 mg/g) and FADB (3.25 ± 0.12 mg/g) than in FDDH ($p < 0.05$).

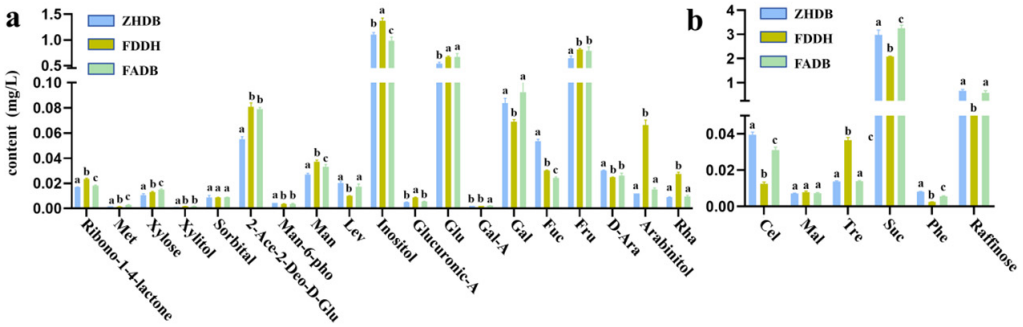

Figure 3. Sugar component content analysis of Baimudan white teas from ZHDB, FADB, and FDDH cultivars. (**a**): Bar plot of monosaccharide component contents. Duncan's test was used to compare whether there were significant differences between the means of two groups. Different letters among groups indicate significant differences at $p < 0.05$. (**b**): Bar plot of disaccharide/polysaccharide component contents.

Flavor thresholds were defined as the minimum concentration required for sensory perception. Sucrose exhibited the lowest sweetness threshold (890 mg/kg), followed by glucose, myo-inositol, *D*-galactose, *D*-sorbitol, and xylitol (1400–6200 mg/kg). In contrast, *D*-arabinitol and raffinose showed considerably higher thresholds (14,000–25,000 mg/kg). Thus, sweetness contributions were determined not only by concentration but also by sensory efficiency. For example, raffinose, despite its relatively high content, contributed minimally due to its elevated threshold. To further clarify the role of soluble sugars, TAVs were calculated (Table 1). Sucrose displayed the lowest threshold and the highest TAV across all cultivars (ZHDB: 3.34; FADB: 3.66; FDDH: 2.33), confirming its dominant role in sweetness perception. All other soluble sugars had TAV values below 1, indicating negligible contributions. However, Pearson correlation analysis between sucrose content and sensory sweetness scores revealed no significant relationship (Supplementary Table S3). This suggests that, while sucrose may establish the baseline sweetness of white tea, differences in perceived sweetness among cultivars are more closely associated with variations in sweet-tasting amino acids, such as serine and asparagine, rather than with sucrose levels. These results highlight sucrose as the principal determinant of sweetness in white tea, with other sugars and amino acids contributing only when present at much higher concentrations.

Table 1. Taste Threshold of Key Flavor Saccharides in Baimudan Tea.

Compounds	Taste Threshold (mg/kg) [26]	Taste Description	ZHDB (TAV)	FADB (TAV)	FDDH (TAV)
Xylitol	3070	Sweet	0.00	0.00	0.00
Sorbitol	6160	Sweet	0.00	0.00	0.00
Inositol	3190	Sweet	0.35	0.31	0.43
Glu	3240	Sweet	0.17	0.21	0.21
Gal	4500	Sweet	0.02	0.02	0.15
D-Ara	17,040	Sweet	0.00	0.00	0.00
Raffinose	14,860	Sweet	0.05	0.04	0.01
Suc	890	Sweet	3.34	3.66	2.33

Note: All threshold values for the listed carbohydrates were determined in an aqueous medium.

3.4. Volatile Aroma Profiling of Baimudan White Tea Processed from Fujian's Primary Cultivars

A total of 380 volatile compounds were identified across the three cultivars, classified into 12 chemical groups: amines (17, 2.6%), alcohols (44, 6.9%), aromatics (37, 5.8%), phenols (10, 1.5%), nitrogen-containing compounds (7, 1.1%), sulfur compounds (5, 0.7%), aldehydes (45, 7.1%), acids (12, 1.9%), terpenoids (177, 18.5%), hydrocarbons (57, 9.0%), ketones (54, 8.5%), esters (107, 16.9%), and heterocycles (107, 16.9%) (Supplementary Table S2). Principal component analysis (Figure 4a) showed that the first two components explained 85.47% of the total variance, clearly separating the three cultivars. Replicates clustered tightly, confirming high experimental reproducibility. Volatile composition analysis revealed that ZHDB was dominated by terpenoids, followed by heterocycles and esters. In contrast, FADB and FDDH exhibited similar profiles, with heterocycles most abundant, followed by terpenoids and esters. ZHDB and FADB contained significantly higher proportions of esters and acids compared with FDDH ($p < 0.05$), while FDDH showed higher levels of hydrocarbons and alcohols. Differential metabolite analysis (Fold Change > 2, $p < 0.05$, VIP > 1) identified 84 significantly different volatiles between ZHDB and FADB, with 77 compounds enriched in ZHDB (Figure 4c). Similarly, 24 and 48 differentially accumulated volatiles were detected between ZHDB vs. FDDH and FADB vs. FDDH, respectively. Key differentially accumulated compounds—including geraniol, trans-limonene oxide, and (*Z*)-3-octen-1-ol—are likely important contributors to aroma differences among the three cultivars.

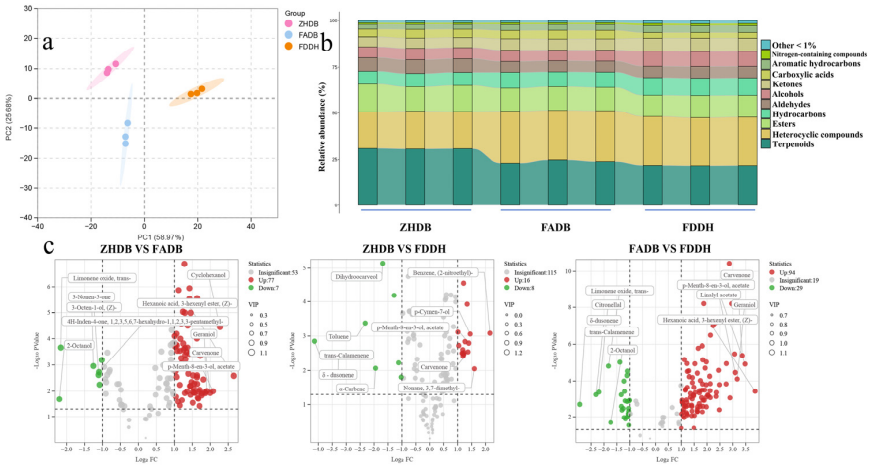

Figure 4. Volatile compound content analysis of Baimudan white teas from Zhenghe Dabai (ZHDB), Fu'an Dabai (FADB), and Fuding Dahao (FDDH) cultivars. (**a**): Principal component analysis (PCA) scatter plot; (**b**): Stacked bar chart showing percentage composition of volatile compound categories in three white tea samples. (**c**): Volcano Plot of Differential Volatile Compounds in Baimudan Tea from ZHDB, FADB, and FDDH). Volcano plot of differential volatile compounds, with thresholds set at $|\log2(\text{fold change})| \geq 1$, VIP value > 1 and p value < 0.05.

3.5. Key Aroma Compounds Determining Sensory Characteristics of Baimudan White Tea

To evaluate the contribution of specific compounds to the overall aroma of white tea, both their concentrations and odor activity values (OAVs) were considered. The OAV is a widely applied metric in flavor research for assessing the relative sensory impact of individual aroma compounds. Compounds with OAVs > 1 are recognized as significantly influencing the overall aroma, while those with OAVs > 10 are regarded as exerting a dominant impact on the tea's aromatic character [27]. OAVs were calculated using reported odor thresholds of each compound in water. Our analysis identified 22 key aroma-active compounds (OAV > 1) across the three Baimudan samples (Table 2). Sweet and fruity notes were primarily attributed to eight sweet compounds, including β-ocimene (OAV 33.4–165.2), benzaldehyde (OAV 21.7–25.7), and geraniol (OAV 281.3–2850.1), together with five fruity compounds such as 1-octanol (OAV 3.1–5.1) and citral (OAV 125.2–152.4). Floral attributes were largely determined by low-threshold compounds including methyl salicylate (OAV 577.7–1732.6), linalool (OAV 4683.8–6387.3), and β-ionone (OAV 1284.1–1541.0). Grassy and fresh notes were derived from LOX pathway intermediates such as (Z)-3-hexenol (OAV 24.2–54.7), (E)-2-hexenal (OAV 70.9–105.4), (Z)-3-hexenal (OAV 2.8–4.8), and hexanal (OAV 333.7–463.1). Elevated levels of these compounds in ZHDB and FADB suggest that they contribute more strongly to the fresh aroma profiles of these cultivars.

Table 2. Quantitative Profile of of Aroma-Active Components in Fujian Baimudan White Tea.

Compounds	Threshold μg/kg [28,29]	Odor Description	ZHDB		FDDH		FADB	
			Content μg/g	OAV	Content μg/g	OAV	Content μg/g	OAV
β-Ocimene	2	Sweet	5.62 a	2808.87	1.14 c	567.75	3.16 b	1581.11
Benzyl alcohol	20,000	Sweet Floral	9.73 a	0.5	8.46 a	0.4	5.68 b	0.3
1-Hexanol	500	Petrol-like	0.99 a	2.0	0.31 b	0.6	0.88 a	1.8
Indole	500	Floral	0.06 a	0.1	0.04 a	0.1	0.03 a	0.1
Benzaldehyde	350	Sweet	9.00 a	25.7	7.60 b	21.7	8.30 a	23.7
Hotrienol	110	Sweet	2.20 a	20.0	2.68 a	24.4	2.62 a	23.9
1-Octanol	110	Fruity	0.54 a	4.9	0.34 b	3.1	0.56 a	5.1
(*Z*)-3-Hexenol	70	Green/Vegetal	3.83 a	54.7	1.69 c	24.2	2.53 b	36.1
Methylsalicylate	40	Floral	69.30 a	1732.6	23.11 c	577.7	48.22 b	1205.4
Geraniol	40	Floral	114.01 a	2850.1	11.25 c	281.3	45.36 b	1134.1
Hexyl hexanoate	40	Fresh	0.12 a	3.0	0.01 b	0.4	0.04 b	1.1
(*E*)-2-Hexenal	17	Green/Vegetal	1.79 a	105.4	1.59 b	93.5	1.20 b	70.9
(*Z*)-3-Hexenal	17	Green/Vegetal	0.07 a	4.4	0.05 a	2.8	0.08 a	4.8
(+)-Limonene	10	Sweet Orange	1.13 a	112.6	0.40 b	40.4	1.01 a	101.1
Linalool	6	Floral	38.32 a	6387.3	28.10 b	4683.8	37.54 a	6257.5
Ionone	5.7	Sweet Floral	0.01 a	1.7	0.01 a	2.4	0.01 a	1.5
Hexyl acetate	5	Apple-like	0.10 a	19.4	0.04 a	7.9	0.06 a	11.7
Hexanal	4.5	Green/Vegetal	1.89 a	419.6	1.50 b	333.7	2.08 a	463.1
β-Ionone	3.5	Floral	4.49 a	1284.1	5.29 a	1510.8	5.39 a	1541.0
β-Cyclocitral	3	Fruity	0.03 a	9.1	0.04 a	14.8	0.03 a	11.3
Citral	3	Fresh Fruity	0.43 a	144.2	0.46 a	152.4	0.38 a	125.2
Myrcene	1.2	Sweet Fatty	4.76 a	3964.3	0.98 c	818.9	3.44 b	2865.1
Pentyl hexanoate	0.05	Sweet Floral	0.09 a	1793.4	0.10 a	2000.3	0.11 a	2206.7

Note: Different lowercase letters in the same row indicate statistically significant differences among the three samples (Duncan's test, $p < 0.05$).

Compounds with OAV values exceeding 10 (Table 2) were identified as the dominant drivers of the aromatic profile, exerting strong sensory effects relative to their concen-

trations. Among these, linalool (OAV 4683.8–6387.3) and β-ionone (OAV 1284.1–1541.0) emerged as the most potent contributors to floral aroma, owing to their exceptionally low thresholds (6 μg/kg and 3.5 μg/kg, respectively). Linalool, β-ionone, methyl salicylate (OAV 577.7–1732.6), and geraniol (OAV 281.3–2850.1) collectively dominated the floral profile, with ZHDB and FADB showing markedly higher concentrations (e.g., linalool at 38.32 μg/g and 37.54 μg/g, respectively, compared with 28.10 μg/g in FDDH). Similarly, (Z)-3-hexenol, hexanal, and (E)-2-hexenal were the principal contributors to green notes. Notably, (Z)-3-hexenol and hexanal were significantly more abundant in ZHDB and FADB, consistent with the more pronounced green/vegetal aroma characteristics of these cultivars. Furthermore, Pearson correlation analysis between the concentrations of key aroma compounds and corresponding sensory aroma attributes revealed significant positive correlations between fresh/green aroma intensity and (Z)-3-hexenol, hexyl hexanoate, (Z)-3-hexenal, and hexanal ($R > 0.85$, $p < 0.05$). Floral aroma intensity was positively correlated with methyl salicylate, geraniol, and linalool ($R > 0.85$, $p < 0.05$), whereas sweet aroma intensity correlated positively with benzyl alcohol ($R > 0.85$, $p < 0.05$) (Supplementary Table S4). In contrast, no significant correlations were found between fruity aroma perception and the concentrations of fruity-associated compounds, which may be attributed to the inherently weak fruity character of Baimudan white tea.

4. Discussion

The relatively simple processing of white tea allows maximum retention of amino acids in fresh leaves, making high amino acid content a defining characteristic of this tea type [30]. Previous studies have demonstrated that amino acids play a central role in shaping tea taste, with white tea containing the highest total amino acid content among the six major tea categories [31]. Moreover, most amino acids in white tea occur at higher levels than in other types [32]. In our analysis, 21 amino acids were detected, with particularly high concentrations of Thea, Asn, Glu, and Gln. These results are consistent with Zhang et al., who analyzed 46 white tea samples and identified Thea and Glu as primary contributors to freshness. Quantitative taste evaluation further confirmed that Thea, Asp, and GABA are the principal umami contributors in white tea [11]. Theanine solution has a caramel-like aroma and a refreshing taste comparable to Glu, but with a much lower taste threshold, making its umami and sweet characteristics more perceptible. Thea also acts synergistically with Glu to enhance umami while reducing bitterness and astringency caused by caffeine and catechins [33], establishing it as a key flavoring substance in tea. In this study, ZHDB and FADB showed higher TAVs for Glu, Asp, and Thea compared with FDDH, consistent with their superior umami scores in sensory evaluation.

Soluble sugars represent another major determinant of tea taste, directly contributing to sweetness [34]. Previous studies reported that soluble sugars not only enhance sweetness but also provide body and roundness to the infusion [35]. In this study, 19 monosaccharides and six polysaccharides were identified, with significant cultivar-specific variations. Concentration differences among varieties are the primary cause of sweetness variability in white tea [26]. However, not all soluble sugars contribute equally. For example, a report showed that among 26 identified soluble sugars, Suc contributes strongly to the sweetness of green, white, yellow, and oolong teas; Glu contributes moderately in black tea; and inositol contributes moderately in white tea. Our results indicated that only Suc significantly influenced sweetness in the tested white teas, while inositol exerted negligible effects, possibly due to differences in cultivar or processing techniques [26]. It is also important to note that tea sweetness does not arise solely from sugars but also from sweet-tasting amino acids such as Thea and Ser [36]. Thea not only imparts umami but also enhances the sweetness of co-existing sugars by interacting with human taste receptors [37]. Although

less abundant than soluble sugars, sweet amino acids modulate flavor through synergistic effects and by masking bitterness and astringency. In this study, Ser and Asn displayed high TAVs across all three cultivars, suggesting both direct and indirect roles in sweetness perception. Thus, the interplay between soluble sugars and sweet amino acids likely forms a complex sweet matrix that explains the observed variation in sweetness among Fujian white tea cultivars.

Relative quantitative analysis of aroma compounds in Baimudan revealed 22 key aroma-active compounds with OAVs greater than 1. The floral attributes of the three white teas were mainly derived from low-threshold compounds such as methyl salicylate, linalool, and β-ionone. Methyl salicylate, a widely distributed aromatic compound in tea, has been shown to form during the withering stage through the activity of salicylic acid carboxyl methyltransferase in *Camellia sinensis*, highlighting its key role in the floral aroma of white tea [38]. Similar findings in black teas further support its role as a floral aroma modifier [39]. It is worth noting that a study on the aroma quality of Zhenghe White Tea found that methyl salicylate is related to the fruity aroma of white tea, which may be due to different concentrations [40]. Linalool, with its distinctive fresh floral scent and very low odor threshold, is another major contributor to tea aroma [14]. Previous studies have also found that linalool is the main contributing component to the floral quality of white tea [41,42]. β-Ionone, a member of the rose ketone family structurally related to damascones and damascenones, imparts a refined floral nuance and is widely associated with the aroma of roses and other flowers [43]. In tea, β-ionone enhances complexity and elegance of the floral profile. It is worth noting that β-Ionone has been identified as the key odorant for different subtypes of white tea, endowing it with an elegant floral quality [44]. Taken together, these findings suggest that methyl salicylate, linalool, and β-ionone act synergistically to shape the characteristic floral aroma of Baimudan white tea.

Previous studies have demonstrated that β-ocimene, benzaldehyde, and geraniol are important contributors to the development of sweet aroma attributes in tea. Among them, geraniol, characterized by its pronounced sweet–floral note, has been identified as the most critical compound shaping the distinctive sweet–floral aroma of Jinguanyin oolong tea [14]. In a study comparing the aromas of fresh white tea with those of aged white tea, it was found that geraniol is the key substance that forms the floral fragrance of white tea, and a relatively high concentration was detected in all white tea samples [45]. Benzaldehyde is considered one of the most representative aromatic aldehydes in tea, known for enhancing fruity and floral characteristics and thereby improving overall sensory quality [14]. β-Ocimene has been reported as a key contributor to the sweet aroma of both oolong tea and Jinmudan black tea, while benzaldehyde has also been identified as a characteristic aroma compound in Hangzhou Gongmei white tea [19,46,47].

(*Z*)-3-Hexenol, (*Z*)-3-hexenal, and (*E*)-2-hexenal, primarily derived from fatty acid degradation, are recognized as major contributors to grassy and fresh-green notes in tea [48]. The contribution of C6 compounds to green notes in white tea is consistently supported across different studies. Our identification of (*Z*)-3-hexenol, (*Z*)-3-hexenal, and (*E*)-2-hexenal as major contributors to grassy and fresh-green notes aligns strongly with findings in other white tea research. The study on white tea similarly reported hexanal, (*E*)-2-hexenal, and (*Z*)-3-hexenol as main contributors to its green note [41]. These compounds are also present in floral-scented green teas, where they impart a fresh, grassy nuance [49]. Notably, fatty acid degradation products often display biphasic odor characteristics: at low concentrations, they provide pleasant fresh-green and brisk aromas, whereas at higher levels, they can introduce undesirable grassy or greenish off-notes [50]. Thus, achieving an appropriate balance of (*Z*)-3-hexenol, (*Z*)-3-hexenal, and (*E*)-2-hexenal is critical for imparting the desirable refreshing aroma associated with white tea. Genetic differences among

tea cultivars lead to variations in the levels of aroma compounds and their precursors in fresh leaves, ultimately shaping cultivar-specific aroma profiles. In this study, compared with FDDH, the higher abundances of methyl salicylate, geraniol, linalool, (*Z*)-3-hexenol, (*Z*)-3-hexenal, and hexanal in ZHDB and FADB appear to be the key chemical determinants underlying their stronger floral and fresh-green aroma characteristics.

The sensory evaluation results for the three cultivars were consistent with the metabolomic findings. ZHDB and FADB, which received significantly higher sensory scores for fresh, floral, and umami attributes, also showed elevated levels of theanine, glutamic acid, and aspartic acid, as well as higher concentrations of low-threshold floral volatiles such as methyl salicylate, linalool, and *β*-ionone. These compounds are well known to enhance freshness, floral aroma, and umami taste in tea infusions. In contrast, FDDH, which scored higher for sweetness, exhibited higher sucrose content, which likely accounts for these sensory characteristics. Such congruence between sensory profiling and chemical composition underscores the cultivar-specific flavor signatures of Baimudan white tea and highlights the chemical basis for their discrimination.

Taken together, our results indicate that cultivars with higher levels of sweet-tasting amino acids and low-threshold floral aroma compounds can enhance desirable sensory traits. The sensory–chemical correlation data can be applied to improve raw material selection and quality grading. From a marketing perspective, these cultivar-specific flavor profiles provide a clear chemical basis for product differentiation, enabling producers to emphasize the natural umami and floral characteristics of certain cultivars in branding and promotion.

5. Conclusions

This study employed an integrative metabolomic approach to elucidate the chemical determinants of flavor quality in Baimudan white teas processed from the three major Fujian cultivars. Sucrose, together with the sweet-tasting amino acids serine and asparagine, was identified as the primary driver of sweetness, while theanine, glutamic acid, and aspartic acid contributed significantly to umami intensity. Floral aroma was predominantly shaped by low-threshold volatiles such as methyl salicylate, linalool, and β-ionone, synergistically complemented by β-ocimene and benzaldehyde. The cultivar-specific accumulation of these compounds accounted for the distinctive sensory characteristics of Zhenghe Dabaicha, Fuding Dahaocha, and Fuan Dabaicha. These findings deepen the understanding of flavor biochemistry in white tea and provide a valuable basis for quality improvement and geographic authentication in the tea industry. However, this study has certain limitations. First, the sample size was relatively small, which may limit the generalizability of the results across broader production regions and harvest years. Second, although key flavor-contributing compounds were identified, their causal roles in perceived aroma and taste were not validated through aroma recombination or spiking experiments. Future work should expand the sampling scope and employ such confirmatory sensory experiments to strengthen the causal links between specific metabolites and flavor perception in white tea.

Supplementary Materials: The following supporting information can be downloaded at: https://www.mdpi.com/article/10.3390/horticulturae11101196/s1, Supplementary Table S1: Sensory evaluation results of the primary cultivar of fujian white tea; Supplementary Table S2: Compound Properties and Peak Area Data. Supplementary Table S3: Correlation matrix between taste attributes and substance content. Supplementary Table S4: Correlation matrix between aroma attributes and substance content. Supplementary Table S5: The boiling points of key aroma substances.

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Informed Consent Statement: The authors ensure that the work described has been conducted in compliance with The Code of Ethics of the World Medical Association (Declaration of Helsinki) for experiments involving humans. The ethical approval of sensory evaluation is not required by national laws. No human ethics committee or formal documentation process is available for sensory evaluation. The authors affirm that appropriate protocols have been used to protect the rights and privacy of all participants. This includes ensuring that participation is voluntary, providing full disclosure of study requirements and risks, obtaining verbal consent from participants, not disclosing participant data without their knowledge, and allowing participants to withdraw from the study at any time.

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