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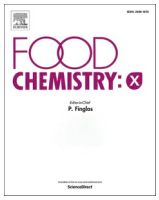

Metabolomics revealed the characteristics of the unique flavor substances of Alxa *Allium mongolicum*

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ABSTRACT

Allium mongolicum is a wild vegetable with high nutritional value and is famous for its taste and aroma. This study used headspace solid-phase microextraction-mass spectrometry coupled with gas chromatography–mass spectrometry techniques to study the metabolic profile of *A. mongolicum* in different ecological environments. A total of 624 volatile organic compounds (VOCs) were identified. Ester compounds, heterocyclic compounds and terpenoids are the key metabolites that determine flavor differences. KEGG analysis showed that monoterpenoid biosynthesis, zein biosynthesis, α-linolenic acid metabolism and secondary metabolite biosynthesis were the most important metabolic pathways. Compared with Minqin *A. mongolicum* and Tengger *A. mongolicum*, Alxa *A. mongolicum* flavor substance notes sensory flavor has more green, fruity, sweet, floral, spicy, metallic, rose, almond, apple, grassy, tropical, citrus, fresh, herbal and other flavor combinations. Overall, this study reveals the main reason for the unique flavor of Alxa *A. mongolicum* through metabolomic evidence.

1. Introduction

Allium is a group of common edible plants, such as *Allium cepa*, *Allium fistulosum* and *Allium tuberosum Rottler ex Sprengle*, which are of great economic value and cultural importance (Şen, Göktürk, Hajiyev, & Uğuzdoğan, 2023; Bi et al., 2024; Wang et al., 2023). The volatile flavor components of allium are mainly composed of aldehydes, alcohols, ketones, acids, phenols, esters, furans and furanones, sulfur and nitrogen, of which sulfur compounds are the main source of the unique flavor of allium (Hao et al., 2023; Kim et al., 2022; Nandakumar et al., 2018). Allium vegetables because of its leaf cells contain volatile sulfides, so it has a pungent smell of volatile oil, can remove the smell of odour and taste, oil and greasy, produce a special aroma, unique aroma and flavor make it a fresh vegetable, processed products and many processed food additives (Kim et al., 2023; Zhang, Jiang, Chen, Sun, & Cui, 2015). Sulfur compounds are characteristic aromatic constituents of allium plants, which have certain pharmacological functions, antibacterial and antifungal effects, can inhibit platelet aggregation, prevent and treat hyperlipidaemia and thrombosis, and significantly reduce blood cholesterol (Richard et al., 2021).

A. mongolicum is widely distributed and mainly grown in Qinghai, Gansu, Xinjiang and Inner Mongolia (Muqier et al., 2017). *A. mongolicum* is a kind of green vegetable without pollution (Zhang, Chen, & Zhang, 2014). *A. mongolicum* contains relatively comprehensive nutrients, mineral nutrients, essential trace elements and amino acids are higher than ordinary vegetables, it is a good companion for cooking various nutritious soups and accompanying meals and wine, and fresh food has a unique flavor (Bu et al., 2023; Wang, Yang, Zhao, & Bao, 2013). Glutamic acid is most abundant in the leaves (Bu et al., 2023; Zhang et al., 2009; Zhang & Ao, 2008). The main constituents of the extract are phenols, aldehydes, ketones, acids, alcohols, thioethers, non-heterocyclic sulfur-containing substances, alkanes, olefins and aromatic hydrocarbons (Lu & Lu, 2002). In addition, *A. mongolicum* offer medicinal benefits, including the ability to regulate functional constipation and to prevent and treat obesity and hypertension (Chen et al., 2020; Wang et al., 2019). As one of the most promising functional foods of the future, demand for *A. mongolicum* is increasing, driving the development of *A. mongolicum* sauce, *A. mongolicum* noodles and other *A. mongolicum* processed foods. However, at the point of sale, Alxa *A. mongolicum* is preferred by consumers. Consumer preference is highly correlated with

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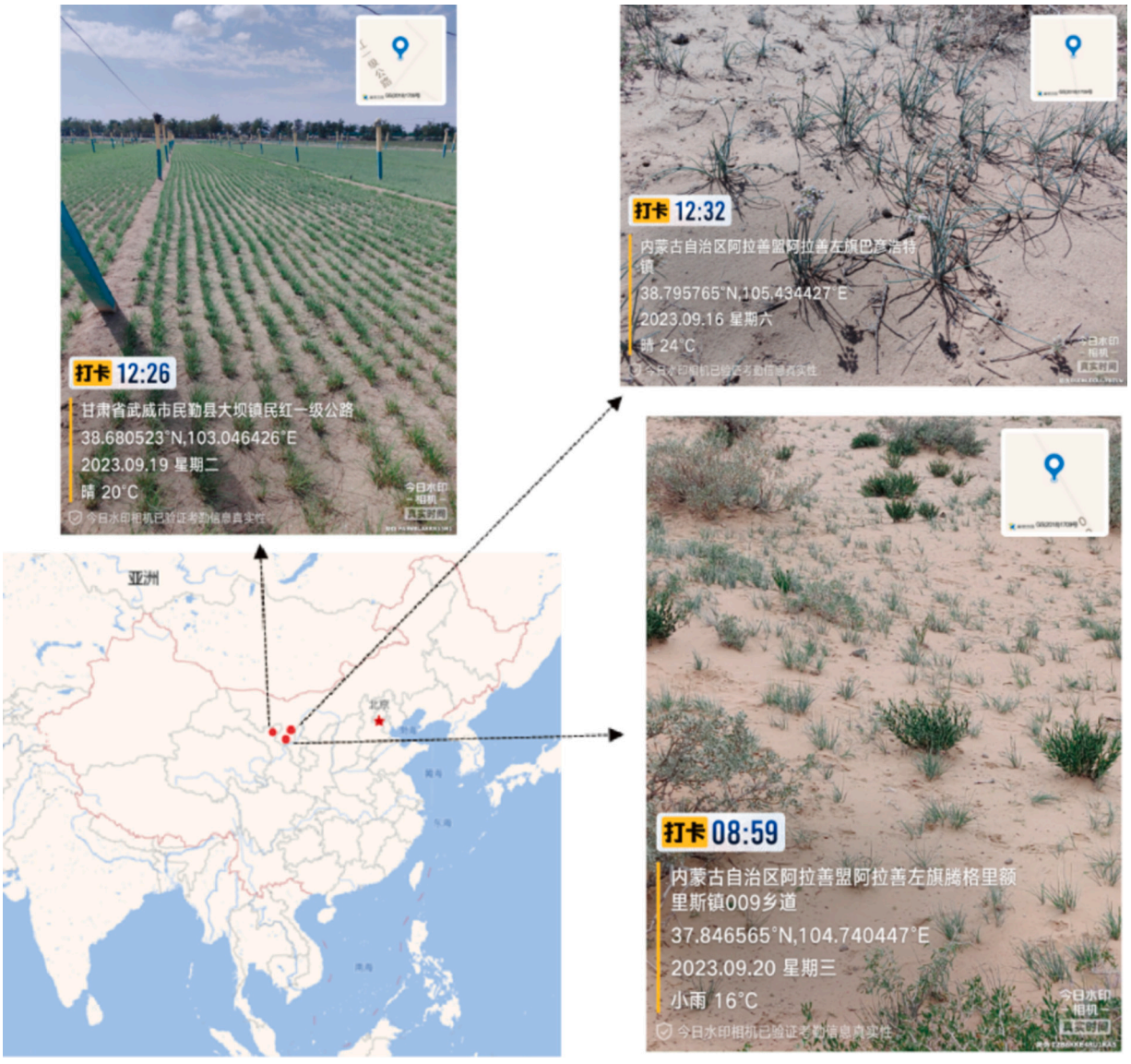

Fig. 1. *A. mongolicum*'s different living conditions.

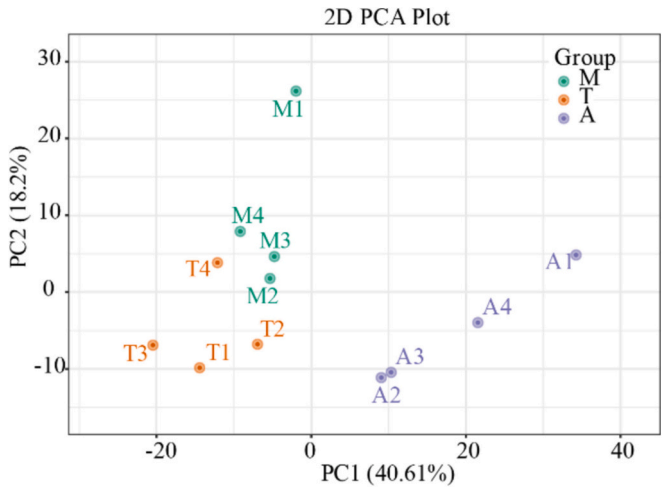

Fig. 2. PCA score of quality spectrum data of each group and quality control samples. The horizontal coordinate PC1 and the vertical coordinate PC2 in the fgure indicate the scores of the frst and second ranked principal components, respectively. The scatter color indicates the experimental grouping of the sample. Each point in the figure represents a sample, and samples from the same group are represented by the same color. A = Alxa *A. mongolicum*, T = Tengger *A. mongolicum*, M = Minqin *A. mongolicum*.

flavor intensity, but GC–MS analysis of flavor metabolite characteristics of Alxa *A. mongolicum* has not been reported.

Metabolomics has become an effective tool to explore the biosynthesis pathway and molecular regulation mechanism of fruit and vegetable flavor chemicals (Baky, Shamma, Xiao, & Farag, 2022; Guo, Li, & Dou, 2024; Nascimento et al., 2019). However, there have been few studies on the flavor compounds of *A. mongolicum*. Therefore, the comprehensive comparison of metabolites of Alxa *A. mongolicum* and *A. mongolicum* from different locations (Tengger *A. mongolicum*, Minqin *A. mongolicum*) will help plant breeders to cultivate and develop varieties with better flavor characteristics.

2. Materials and methods

2.1. Materials

The fresh samples of *A. mongolicm* were collected from Alxa league, around the Tengger Desert, and Minqin, Gansu, in September 2023 (Fig. 1). Identified by Prof. ZhongRen Yang of Inner Mongolia Agricultural University (IMAU). A voucher specimen (No. 20230930–001) was deposited at the College of Horticultural and Plant Protection of IMAU.

2.2. Sample preparation and GC–MS analysis

The powder was processed according to the method of Wang et al. (2023). Volatile organic compounds (VOCs) of *A. mongolicum* were determined by Wuhan Metware Biotechnology Co., LTD. (Wuhan, China, http://www.metware.cn/) based on the Agilent 7890B—7000D platform at 250 °C in splitless mode (flow rate 1 ml /min). The detection time was 5 min. Each experiment was repeated 4 times. 1 g of the powder was transferred into a 20 ml headspace vial (Agilent, CA, USA) containing 2 ml NaCl saturated solution to inhibit any enzyme reaction. Each vial was oscillated at 60 °C for 5 min, and a 120 μm DVB/CWR/PDMS extraction head was inserted into the sample headspace vial for 15 min. It was analyzed at 250 °C for 5 min, and then isolated and identified by GC–MS/MS (7890B gas chromatography and 7000D mass spectrometer (Agilent, CA, USA). Helium (99.999 %) was used as the carrier gas and the carrier gas flow rate was 1.0 ml/min. Maintain syringe temperature at 250 °C and detector temperature at 280 °C. The mass spectrometry (MS) was performed in electron shock (EI) ionization mode at 70 eV, with a scan range of *m/z* 20–550 amu at 1 s intervals. The quadrupole mass detector, ion source and transmission line temperatures are set at 150 °C, 230 °C and 280 °C respectively. Volatile compounds were identified by mass spectrometry compared with NIST database and linear retention index (Li et al., 2021).

2.3. Relative odour activity value (rOAV) analysis of metabolites

rOAV analysis according to the method of Huang et al. (2023). rOAV is a method of determining the major flavor compounds in foods based on the sensory threshold of the compounds and is used to clarify the contribution of each flavor compound to the overall flavor characteristics of the sample.

In general, rOAV ≥1 indicates that the compound makes a direct contribution to the flavor of the sample.

2.4. Data analysis

Unsupervised principle component analysis (PCA) was performed using the statistical function prcomp in R v3.5.0 (www.r-project.org). Supervised multiple regression orthogonal partial least squares discriminant analysis (OPLS-DA) was performed using ropls v1.19.8 in R (Chong & Xia, 2018). We used the threshold variable importance (VIP) value (VIP ≥ 1.0) in the OPLS-DA model to screen for these differential metabolites. To assess the significance of differences in metabolite abundance, a Student's *t*-test (mean two-tailed) was used ($p = 0.05$). Annotated metabolites were mapped to the Kyoto Encyclopedia of Genes and Genomes (KEGG) pathway database (http://www.kegg.jp/kegg/pathway.html) to determine pathway associations. Pathway enrichment analysis was performed on the web-based Sever Metabolite Sets Enrichment Analysis (MSEA; http://www.msea.ca). Bonferroni-corrected pathways with a *P* value ≤0.05 were considered significantly enriched.

3. Results

3.1. Overview of metabolic profiles

3.1.1. Volatile organic compounds (VOCs) in A. mongolicum.

In order to detect the diversity of metabolites, HS-SPMEGC/MS technology was used to analyze volatile organic compounds in samples of *A. mongolicum*. A total of 624 metabolites were identified based on GC–MS detection platform and self-built database. Among them, terpenoids (102), ketones (44), hydrocarbons (66), alcohols (36), acids (15), esters (111), aldehydes (49), aromatics (38), heterocyclic compounds (106), sulfur-containing compounds (8), other classes (6), amines (20), halogenated hydrocarbons (4), nitrogen-containing compounds (6), ethers (2), phenols (11). Among them, esters contributed the most (17.79 %), followed by heterocyclic compounds (16.99 %) and terpenoids (16.35 %), which were the main components of volatile organic compounds of *A. mongolicum* in this study (Table S1). These results indicated that ester compounds, heterocyclic compounds and terpenoids were the most abundant metabolites in *A. mongolicum*.

3.1.2. Principal component analysis (PCA)

To illustrate the presence of flavor substances in different habitats, we analyzed the metabolic profiles of 624 identified metabolites using PCA (Fig. 2). The first principal component (PC1) explained 40.61 % of the metabolic differences among the three habitats, and the second principal component (PC2) explained 18.2 % of the metabolic differences among the three habitats. On PC1, group A was separated from group T and group M, which showed that the content of flavor substances in the samples of Alxa *A. mongolicum*, Tengger *A. mongolicum* and Minqin *A. mongolicum* etes was different. At the same time, the differential accumulation of volatile organic compounds is of great significance to elucidate the aroma formation mechanism of *A. mongolicum*.

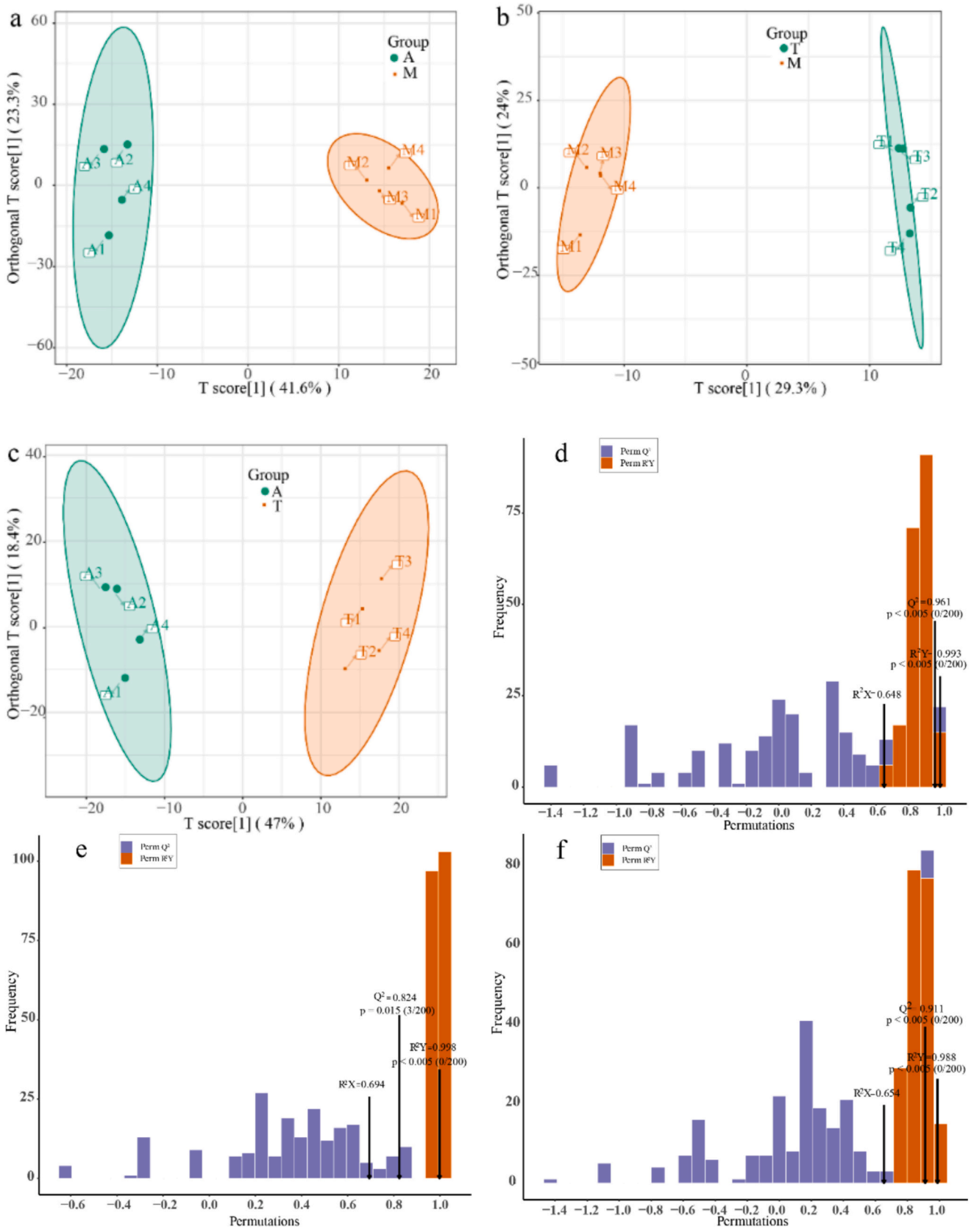

Fig. 3. OPLS-DA scores. Scores of the OPLS–DA model with (a) A vs M, (b) T vs M, (c) A vs T. The permutation test chart for OPLS–DA model. The abscissa represents the model accuracy, and the ordinate is the frequency of the model classification effect. (d) A vs M, (e) T vs M, (f) A vs T. A = Alxa *A. mongolicum*, T = Tengger *A. mongolicum*, M = Minqin *A. mongolicum*.

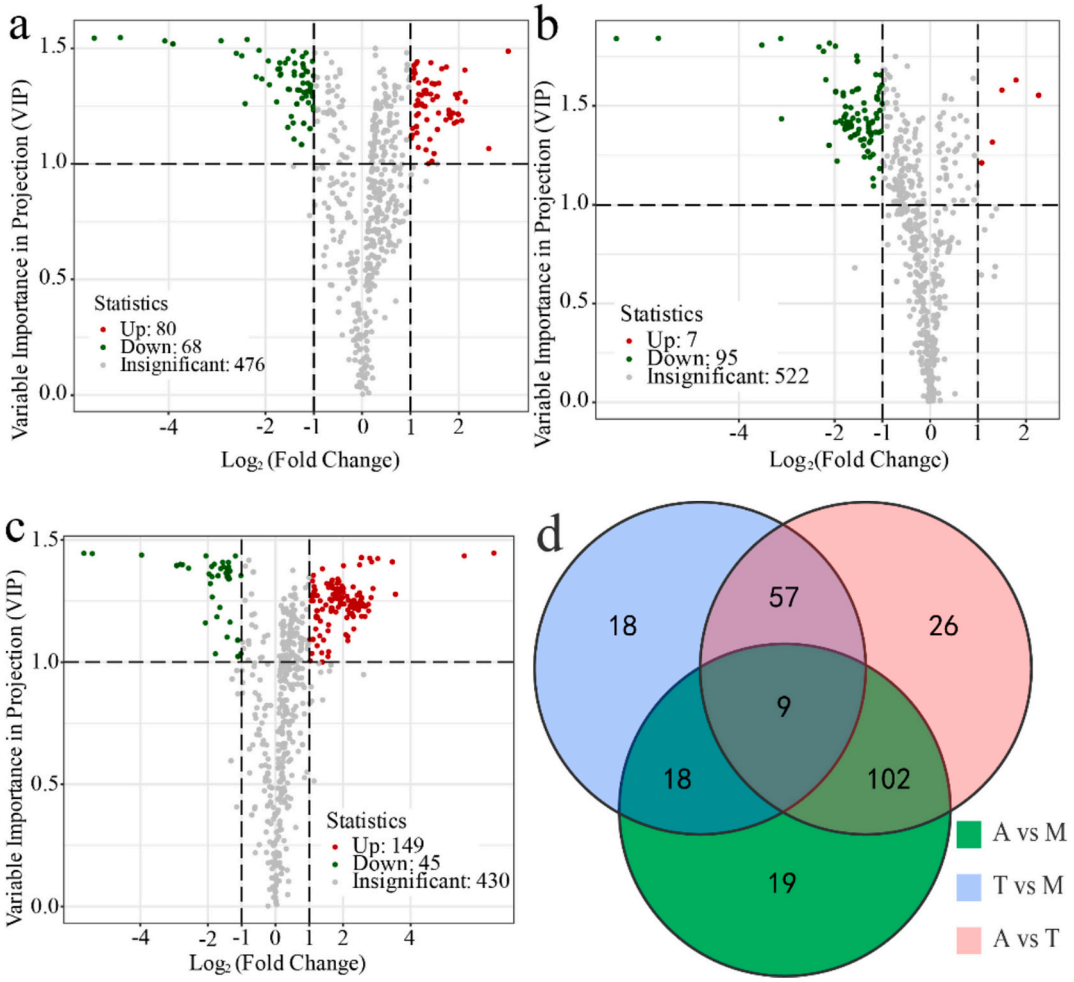

Fig. 4. Volcano plot (a, b, c)and Venn diagram (d) of differential VOCs in *A. mongolicum.* (a) A vs M, (b) T vs M, (c) A vs T. A = Alxa *A. mongolicum*, T = Tengger *A. mongolicum*, M = Minqin *A. mongolicum.*

Therefore, these differentially expressed VOCs were analyzed in detail in this study.

3.1.3. Orthogonal partial least squares discriminant analysis (OPLS-DA) and OPLS-DA model validation

PCA analysis methods cannot ignore within-group errors and cannot exclude random errors. To further determine the differences in Volatile organic compounds (VOCs) under different growing conditions of *A. mongolicum*, we used supervised OPLS-DA analysis on different growing conditions of *A. mongolicum* (Fig. 3a-c). As can be seen from the score plot, the samples from the different treatment groups were effectively differentiated, and unlike the PCA results, the degree of aggregation within each group was more aggregated than in the PCA method.

According to the model established by OPLS-DA, Q2 values were greater than >0.8(Fig. 3d-f), and there is no overfitting phenomenon, indicating that OPLS-DA has a high separation ability in this study.

3.2. Differential metabolite analysis

3.2.1. Differential metabolite screening

Based on VIP of OPLS-DA model, we found that there were significant differences in VOCs variance among different producing areas. Then, we further screened differential metabolites, with specific screening conditions as follows: fold change≥2 or fold change≤0.5, VIP ≥ 1, p value <0.05, a total of 249 differential metabolites were screened (Table S2), and these differential metabolites came from 15 types of substances, among which esters (n = 40) accounted for the largest proportion. Followed by terpenoids (n = 39), heterocyclic compounds (n = 38), hydrocarbons (n = 22), ketones (n = 20), aldehydes (n = 20), aromatics (n = 17), alcohols (n = 16), amines (n = 14), sulfur-containing compounds (n = 6), phenols (n = 6), acids (n = 5), others (n = 4), halogenated hydrocarbons (n = 1), and ethers (n = 1). Compared with Minqin *A. mongolicum*, 148 metabolites (80 up-regulated and 68 down-regulated) were found in Alxa *A. mongolicum* (Fig. 4a), 102 metabolites (7 up-regulated and 95 down-regulated) were found in Tengger *A. mongolicum* (Fig. 4b). Compared with Tengger *A. mongolicum*, 194 metabolites (149 up-regulated and 45 down-regulated) were found in Alxa *A. mongolicum* (Fig. 4c), indicating that more volatile substances accumulated in Alxa *A. mongolicum* than in Minqin *A. mongolicum* and Tengger *A. mongolicum*, and the different-expressed VOCs may be an important factor in the aroma formation of Alxa *A. mongolicum*. Detailed analysis showed that compared with Minqin *A. mongolicum*, the 80 VOCs significantly accumulated by Alxa *A. mongolicum* were mainly esters (15 kinds), followed by terpenoids (14 kinds), heterocyclic compounds (14 kinds) and aromatics (8 kinds). Compared with Tengger *A. mongolicum*, terpenoids (27 kinds) were the main VOCs accumulated in 149 VOCs, followed by esters (25 kinds), heterocyclic compounds (23 kinds) and hydrocarbons (13 kinds). From Venn diagram (Fig. 4d), it can be seen that Alxa *A. mongolicum* and other local *A. mongolicum* share common metabolites and some unique metabolites. However, it is interesting to note that terpenoids and esters accounted for a small proportion of significantly down-regulated VOCs, while aldehydes accounted for a large proportion. The significantly upregulated terpenoids and esters are (1-Oxaspiro[4.5]dec-6-ene, 2,6,10,10-tetramethyl-), (Bicyclo[3.1.0]

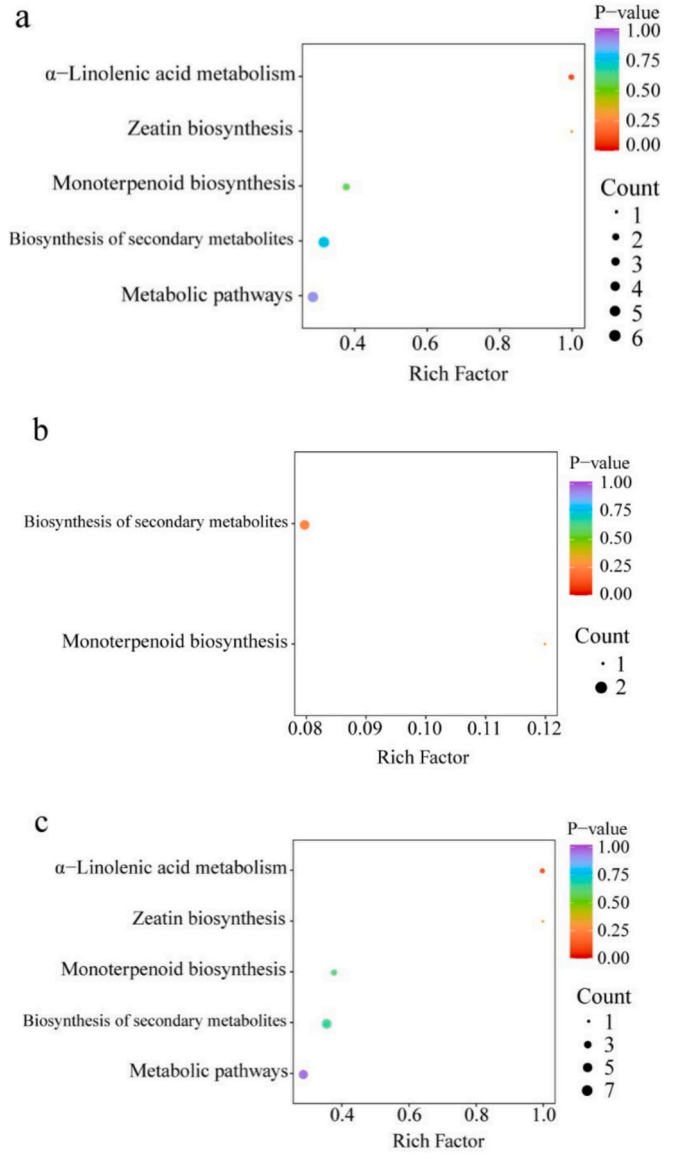

Fig. 5. KEGG enrichment map of differential VOCs of *A. mongolicum* under different growing conditions.
(a) A vs M, (b) T vs M, (c) A vs T. A = Alxa *A. mongolicum*, T = Tengger *A. mongolicum*, M = Minqin *A. mongolicum*.

hex-3-en-2-one, 4-methyl-1-(1-methylethyl)-), (Propanoic acid, butyl ester), (Cis-cyclohexanone, 5-methyl-2-(1-methylethyl)-), (Diethyl malonate), (Propanoic acid, 2-methyl-, phenylmethyl ester), (Butanoic acid, 2-methyl-, 2-methylbutyl ester), etc. The results indicated that terpenoids and esters might be the key substances for good flavor of Alxa *A. mongolicum*.

3.2.2. KEGG pathway analysis of differential metabolites

We mapped these 249 metabolites to the KEGG database, and conducted pathway enrichment analysis of the metabolites significantly expressed in different habitats of the *A. mongolicum*, and identified the main pathways involved in these metabolites.

Compared with Minqin *A. mongolicum*, the main pathways of flavor substances significantly enriched in Alxa *A. mongolicum* were monoterpenoid biosynthesis (3 metabolites), secondary metabolites biosynthesis (8 metabolites), zeatin biosynthesis (1 metabolite), α-linolenic acid metabolism (2 metabolites), metabolic pathways (8 metabolites), etc. (Fig. 5a).

Compared with Minqin *A. mongolicum*, the main pathways of flavor substances significantly enriched in Tengger *A. mongolicum* were monoterpenoid biosynthesis (1 metabolite) and biosynthesis of secondary metabolites (2 metabolites), etc. (Fig. 5b).

Compared with Tengger *A. mongolicum*, the main pathways of flavor substances significantly enriched in Alxa *A. mongolicum* were monoterpenoid biosynthesis (3 metabolites), biosynthesis of secondary metabolites (9 metabolites), zeatin biosynthesis (1 metabolite), α-linolenic acid metabolism (2 metabolites), metabolic pathways (8 metabolites), etc. (Fig. 5c). Obviously, the differential metabolites cis-3-Hexenol and cis-3-Hexenal of Alxa *A. mongolicum* were significantly enriched in α-linolenic acid metabolism level compared with Minqin *A. mongolicum* and Tengger *A. mongolicum* (Table S2).

3.2.3. Analysis of sensory flavor characteristics of differential VOCs.

A. mongolicum is widely consumed for its unique flavor and nutritional value. Flavor components can objectively reflect the flavor characteristics of different samples and are important indexes for evaluating flavor quality. Sensory analysis of *A. mongolicum* can be used to further understand their contribution to overall flavor. Make use of these databases of odour sensory information (https://www.odour.org.uk; https://www.flavornet.org; https://www.femaflavor.org/flavor-library), The 249 differential metabolites obtained by screening were annotated to sensory flavor features, and the top 10 sensory flavors with the highest number of annotations were selected to draw the radar map (Fig. 6).

Compared with Minqin *A. mongolicum*, there are 140 sensory flavors annotated by flavor substances of Alxa *A. mongolicum*. The main flavors are green (25), fruity (22), sweet (21), floral (8), spicy (8), metallic (7), rose (7), almond (6), apple (6), grassy (6); Among them, spicy and sweet substances are listed in Table 1 (A vs M). Compared with Tengger *A. mongolicum*, there are 156 sensory flavors annotated by flavor substances of Alxa *A. mongolicum*. The main flavors are green (34), fruity (25), sweet (25), tropical (11), citrus (9), floral (9), spicy (9), apple (8), fresh (8), herbal (8); Among them, spicy and sweet substances are listed in Table 1 (A vs T). Compared with Minqin *A. mongolicum*, there are 98 kinds of sensory flavors annotated by flavor substances of Tengger *A. mongolicum*. The main flavors are fruity (15), green (14), sweet (11), tropical (7), herbal (6), roasted (6), apple (5), banana (5), citrus (5), fatty (5); Among them, spicy and sweet substances are listed in Table 1 (T vs M). Therefore, more volatile substances were accumulated in Alxa *A. mongolicum* than in Minqin *A. mongolicum* and Tengger *A. mongolicum*, and the overlaps of differently expressed volatile organic compounds might explain the unique flavor formed by Alxa *A. mongolicum*.

4. Discussion

As a characteristic vegetable with unique flavor and high nutritional value in desert, *A. mongolicum* is commonly used to please seasoning and assisted to cook delicious dish, providing health benefits to human body (Wang et al., 2019). Alxa *A. mongolicum* had high levels of total amino acids and umami amino acids. Principal component analysis revealed a strong correlation between the sweet and savoury characteristics of *A. mongolicum* and the presence of sweet free amino acids, suggesting that *A. mongolicum* have a significant advantage in flavor development (Hou, 2020). Esters, aldehydes and sulfur compounds were found to be the main volatile oil components in *A. mongolicum* (Liu, Zhao, & Yang, 2007; Wuren, 2011). Previous studies have shown that different extraction conditions and the selection of extraction head will affect the incompatibility of peak surface abundance and polarity of volatile components, which easily leads to the instability of component determination (Li et al., 2019). Wang et al. detected a total of 24 compounds by headspace solid-phase microextraction combined with GC, and the volatile components were mainly 2-hexenal and thioether (Wang, Yang, & Bao, 2012). Wen et al. identified a total of 31 compounds by supercritical fluid extraction and Soxhlet extraction (Wen, Liu, & Gao, 2018).

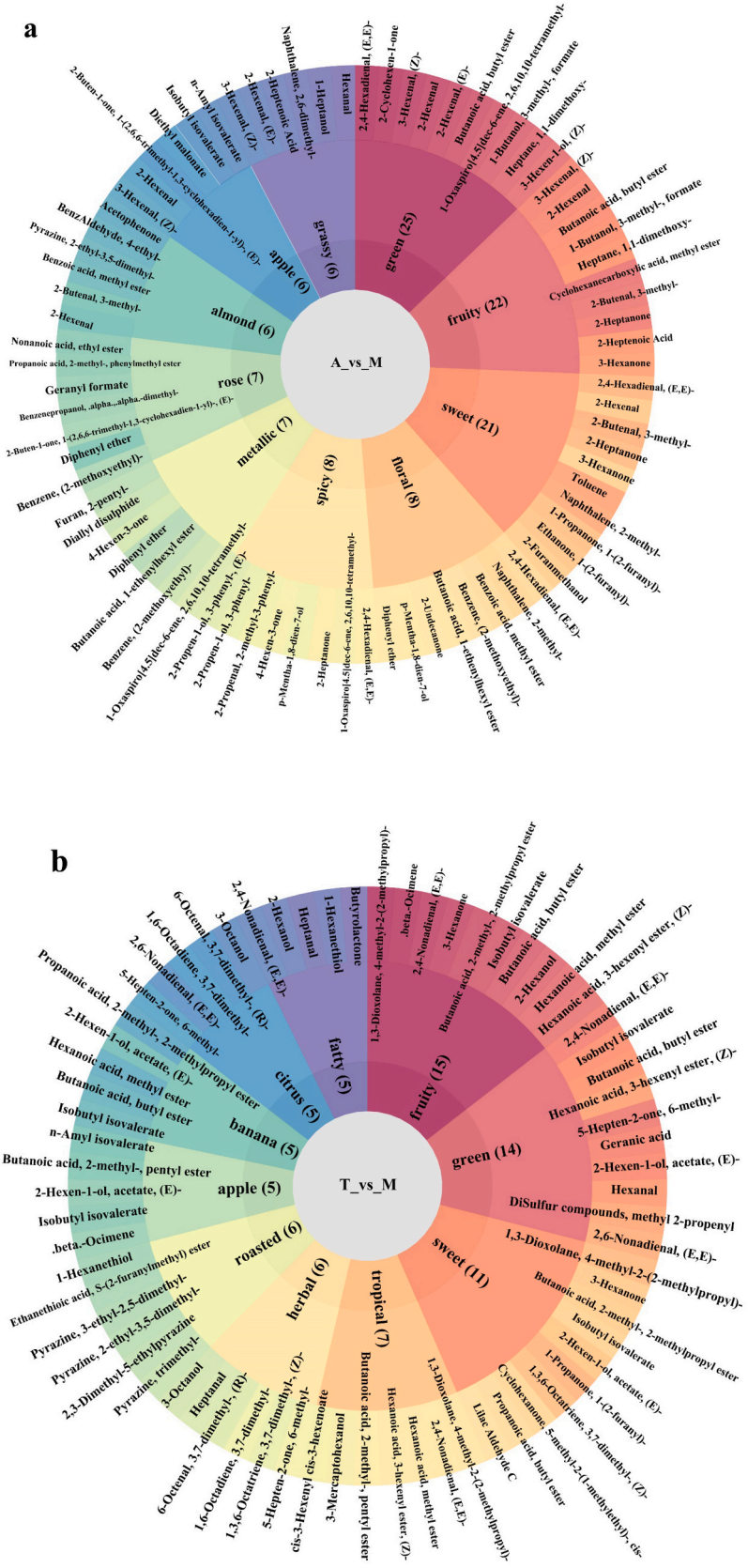

Fig. 6. Analysis of sensory flavor characteristics of differential VOCs
(a) A vs M, (b) T vs M, (c) A vs T. A = Alxa *A. mongolicum*, T = Tengger *A. mongolicum*, M = Minqin *A. mongolicum*.

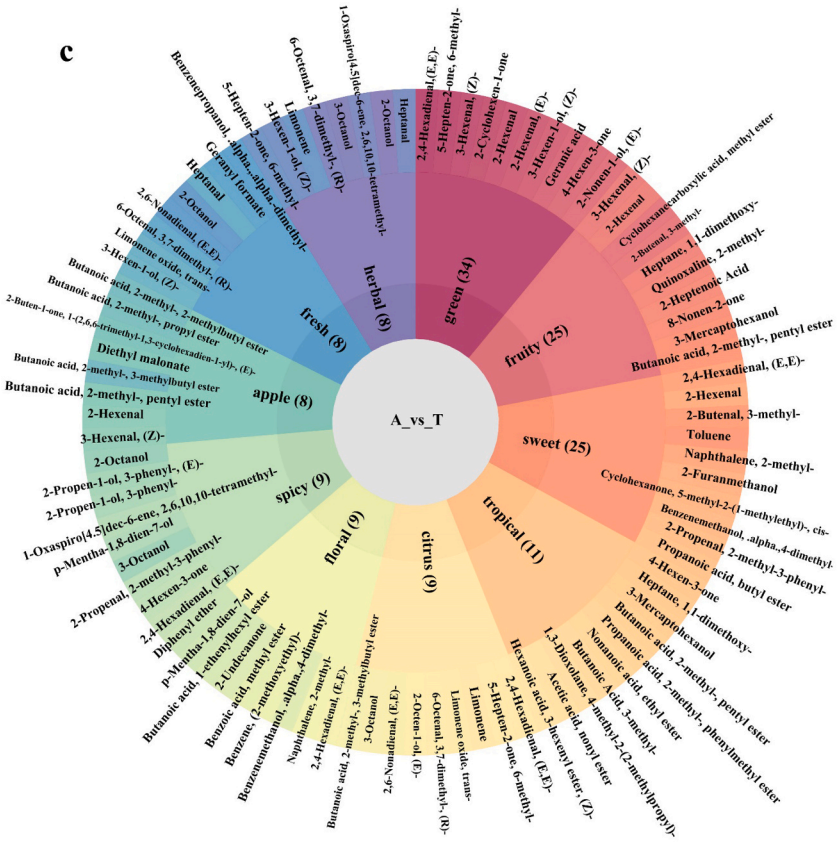

Fig. 6. (*continued*).

Considering the instability and influence of traditional extraction methods on the detection results, some scholars turned to headspace solid phase microextraction (HS-SPME) combined with gas chromatography–mass spectrometry to study the volatile components of plants, and the detection results were relatively stable (Hou, 2020). In this study, a total of 624 volatile compounds were identified from three habitats by HS-SPMEGC/MS analysis (Table S1). Obviously, different extraction methods affect the types of volatiles. This may be due to the extremely complex composition of flavor substances, volatile substances are unstable and different experimental processes will greatly affect the experimental results (Shi, 2008). The results of principal component analysis showed that metabolites of different species and varieties had different characteristics. The OPLS-DA model with high R^2Y and Q^2 values is established. This study provides metabolic evidence for understanding flavor differences in *A. mongolicum*.

Flavor is one of the most relevant factors for consumers to evaluate quality, and their purchase preferences are related to both consumer evaluation quality and their purchase preferences. Lkhagvasuren determined the alliin content of *A. mongolicum* in different producing areas and found that the alliin content of *A. mongolicum* planted in Inner Mongolia was the highest, which was 29.8 mg/g, while the alliin content of *A. mongolicum* planted in Gansu was 15.8 mg/g (Lkhagvasuren, 2020). Flavor substance is a mixture of different volatile substances, including alcohols, aldehydes, ketones, terpenoids, esters and sulfur compounds, etc., which show the aromatic characteristics of a certain vegetable product (Liu, Hao, & Tang, 2008). Suo et al. revealed changes in flavor quality by metabolomics, with terpenoids showing a gradual accumulation pattern (Suo et al., 2023). Zhang et al. identified 119 volatile compounds in coriander by GC–MS, with the highest content of aldehydes (Zhang et al., 2024). Changes in the volatile compounds of peppers during the drying process based on HS-GC–MS was studied by Ge et al. (2020). Zhang et al. studied the effect of drying methods on volatile compounds of *A. mongolicum* based on headspace gas chromatography mass spectrometry (Zhang, Cao, Li, & Wang, 2022). Sulfur compounds are the main source of the characteristic flavor of Green onion (Kim et al., 2022; Nandakumar et al., 2018). Different volatile components give people different flavor perception. Fang et al. (2018) believed that compounds with different aroma groups and different carbon chain structures contributed different degrees to the aroma of scallions. Tian, Yu, Wang, and Li (2016) found that different volatile components of different scallions had different aromas. Hou (2020) and Wen et al. (Wen, Liu, Gao, & Li, 2016) found that the content of sulfur compounds in the Gansu population was 0, which was different from the results of this experiment, and may be caused by different extraction methods. Hou (2022) found that the contents of total amino acids and umami amino acids in Alxa Zuoqi population of Inner Mongolia were higher than those in other 3 populations. In this study, it was found that the sweet-like substances that contributed most to odour in Alxa *A. mongolicum* population were higher than those in other 2 populations. Such as ((E,E)-2,4-Hexadienal), (2-Heptanone), (4-Hexen-3-one), (1-Oxaspiro[4.5]dec-6-ene, 2,6,10,10-tetramethyl-), (2-Propen-1-ol, 3-phenyl-), (3-Phenyl-2-propen-1-ol), (2-Propenal, 2-methyl-3-phenyl-), (p-Mentha-1,8-dien-7-ol), etc. This also explains why Alxa *A. mongolicum* have some unique sweet flavors compared to others. Therefore, Alxa *A. mongolicum* possesses a significant advantage in flavor development.

5. Conclusion

In this study, a wide range of targeted GC–MS metabolomics analysis was used to compare the differences in the metabolic profiles of different habitats, and a total of 624 metabolites were found. Among them, esters, heterocyclic compounds and terpenoids may be related to the flavor of *A. mongolicum*. Further KEGG enrichment analysis of 249 differentiated

Table 1
The difference in the spiciness and sweetness of the *A. mongolicum* in different locations.

	A vs M	A vs T	T vs M
Spicy substances	(E,E)-2,4-Hexadienal) , (2-Heptanone) , (4-Hexen-3-one) , (1-Oxaspiro[4.5]dec-6-ene,2,6,10,10-tetramethyl-) , (2-Propen-1-ol, 3-phenyl-) , (3-Phenyl-2-propen-1-ol) , (2-Propenal, 2-methyl-3-phenyl-) , (p-Mentha-1,8-dien-7-ol)	((E,E)-2,4-Hexadienal) , (4-Hexen-3-one) , (2-Octanol) , (1-Oxaspiro[4.5]dec-6-ene, 2,6,10,10-tetramethyl-) , (2-Propen-1-ol, 3-phenyl-) , (3-Phenyl-2-propen-1-ol) , (2-Propenal, 2-methyl-3-phenyl-) , (p-Mentha-1,8-dien-7-ol) , (3-Octanol).	3-Octanol
Sweet substances	(1-Propanone, 1-(2-furanyl)-) , ((E,E)-2,4-Hexadienal) , (2-Butenal, 3-methyl-) , (2-Furanmethanol) , (2-Heptanone) , (2-Hexenal) , (3-Hexanone) , (4-Ethylbenzaldehyde) , (2-Acetylfuran) , (2-Methylnaphthalene) , (Toluene) , ((E)-2-Buten-1-one, 1-(2,6,6-trimethyl-1,3-cyclohexadien-1-yl)-) , (2-Propen-1-ol, 3-phenyl-) , (3-Phenyl-2-propen-1-ol) , (2-Propenal, 2-methyl-3-phenyl-) , (Acetophenone) , (BenzAldehyde, 3-methyl-) , (Butanoic acid, 2-methyl-, 2-methylpropyl ester) , (Diethyl malonate) , (Isobutyl isovalerate) , (Propanoic acid, 2-methyl-, phenylmethyl ester).	(1,3-Dioxolane, 4-methyl-2-(2-methylpropyl)-) , ((E,E)-2,4-Hexadienal) , (2-Butenal, 3-methyl-) , (2-Furanmethanol) , (2-Hexenal) , (4-Ethylbenzaldehyde) , (2-Methylnaphthalene) , (Toluene) , (Lilac Aldehyde C) , (Lilac Aldehyde D) , ((E)-2-Buten-1-one, 1-(2,6,6-trimethyl-1,3-cyclohexadien-1-yl)-) , (2-Propen-1-ol, 3-phenyl-), (3-Phenyl-2-propen-1-ol), (2-Propenal, 2-methyl-3-phenyl-), (Acetophenone), (BenzAldehyde, 3-methyl-), (Diethyl malonate), (Propanoic acid, 2-methyl-, phenylmethyl ester), (2H-Pyran-2-one, tetrahydro-), (Benzenemethanol, .alpha.,4-dimethyl-), (Butanoic acid, 2-methyl-, 2-methylbutyl ester), (Butanoic acid, 2-methyl-, 3-methylbutyl ester), (Butanoic acid, 3-methyl-, 3-methylbutyl ester), (cis-menthone), (Propanoic acid, butyl ester).	(1-Propanone, 1-(2-furanyl)-), (3-Hexanone), (Butanoic acid, 2-methyl-, 2-methylpropyl ester), (Isobutyl isovalerate), (1,3-Dioxolane, 4-methyl-2-(2-methylpropyl)-), (cis-menthone), (Lilac Aldehyde C), (Lilac Aldehyde D), (Propanoic acid, butyl ester), ((Z)-1,3,6-Octatriene, 3,7-dimethyl-), ((E)-2-Hexen-1-ol, acetate)

metabolites showed that moniterpenoid biosynthesis, zein biosynthesis, α-linolenic acid metabolism and secondary metabolite biosynthesis were the key metabolic pathways. Flavor wheel analysis showed that compared with Minqin *A. mongolicum* and Tengger *A. mongolicum*, Alxa *A. mongolicum* flavor substance notes had more sensory flavors: green, fruity, sweet, floral, spicy, metallic, rose, almond, apple, grassy; tropical, citrus, fresh, herbal and other flavor combinations. The results of this study will enrich the chemical information of aroma composition and aromatic compound formation of *A. mongolicum*, provide evidence for the flavor of *A. mongolicum*, and provide a useful basis for the breeding and processing of *A. mongolicum* to regulate aromatic compounds.

CRediT authorship contribution statement

Dong Zhang: Writing – original draft. **Fenglan Zhang:** Validation, Resources. **Xiaoyan Zhang:** Conceptualization. **Zhenyu Cao:** Software, Investigation. **Xiaoqing Song:** Formal analysis, Data curation. **Tong Zhang:** Methodology, Formal analysis, Data curation, Conceptualization. **Zhongren Yang:** Project administration.

Declaration of competing interest

We declare that we have no financial and personal relationships with other people ororganizations that can inappropriately influence our work, there is no professional or otherpersonal interest of any nature or kind in any product, service and/or company that could beconstrued as influencing the position presented in, or the review of, the manuscript entitled. 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.

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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.2024.101979.

Data availability

Data will be made available on request.

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