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Advances and Perspectives in Fruits and Vegetables Flavor Based on Molecular Sensory Science

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ABSTRACT
Fruits and vegetables contain a large number of volatile compounds, which constitute their unique odor and contribute to their flavor. However, there are only a few key aroma compounds that contribute to the special aroma. How to screen and identify key aroma compounds from many non-contributing and low-contributing compounds has always been the focus and difficulty of the research on the flavor quality of fruits and vegetables. However, it could be better solved via molecular sensory science technology. This review summarizes the application of molecular sensory science technology in fruits and vegetables flavor in recent years, and elaborates the analysis methods related to molecular sensory science, such as sensory evaluation, GC×GC-MS,GC-IMS, GC-O, OAV, omission test and recombination experiment. And some problems existing in current molecular sensory science technology are discussed and prospected.

KEYWORDS
Flavor; molecular sensory science; sensory evaluation; GC×GC-MS; GC-IMS; GC-O

Introduction

Flavor profile can stimulate people's perception and psychology, and then promote consumer acceptance of vegetable and fruit.[1] Aroma has a significant effect on the overall flavor of fruits and vegetables, which is a complex mixture of volatile compounds. Therefore, research on the flavor quality will not only help resource mining and variety cultivation of high-quality flavor fruits and vegetables, but also have important reference and guiding significance for the production and consumption. To date, numerous compounds have been identified from the volatile components of fruits and vegetables.[12] Only a part of the volatile components could contribute special aroma to the fruits and vegetables, making it play a major role in the presentation of the aroma characteristics of the fruits and vegetables. Volatile components with this property are called odor active compounds or key aroma compounds.[3] Therefore, how to screen and identify key aroma compounds from many non-contributing and low-contributing compounds has always been the focus and difficulty of the research on the flavor quality of fruits and vegetables. During the processing of fruits and vegetables, off-flavor may be caused due to improper process conditions or heating.[4–7] Off-flavor substances will cause the aroma of fruit and vegetable products to be inconsistent, thereby affecting the quality of the products. Therefore, clarifying the off-flavor substances in the products and exploring the formation mechanism during the processing has important practical significance for better control and improvement of the flavor quality of fruits and vegetables.

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Molecular sensory science technology, which is proposed by Professor Peter Schieberle in 2007,[8] provides a better way to identify the key aroma compounds and clear the off-flavor of fruits and vegetables and their products. Molecular sensory science is often based on GC-MS and GC-O, combined with OAV, omission test and aroma reconstitution experiment to qualify, quantify and describe the flavor at the molecular level, and accurately construct the flavor recombination of food to determine flavor composition in food. After years of development, molecular sensory science has become the most advanced systematic application technology in flavor analysis of fruits and vegetables and their products.

Molecular sensory science is a systemic science that combines instrumental analysis with sensory evaluation. This review will elaborated the analysis techniques such as GC×GC-MS, GC-IMS, GC-MS, GC-O, OAV and sensory evaluation, and have a perspective on development directions of the future research on the flavor quality of fruits and vegetables.

Sensory evaluation of flavor and application

Sensory analysis is a combination of sensory assessors' visual, olfactory, taste and other sensory organs to evaluate the sensory attributes of food, and combines physiological, psychological, chemical and statistical analysis to evaluate consumers' preference.[9] In the volatile aroma research, sensory analysis refers to people's perception of the volatile substances in food through olfactory.

Sensory evaluation methods mainly include difference test method, descriptive analysis method, and consumer test.[10] The descriptive analysis method is the most widely used in food sensory analysis. It can accurately analyze the differences between the sensory characteristics of different samples, and obtain consumers' detailed perception of sample attributes, thereby improving the quality of samples.[10]

Sensory evaluation was mainly used for discriminating the different aroma of fruits and vegetables, and to identify the properties of aroma compounds.[11,12] Krumbein and Laboissière analyzed aroma of different tomato cultivars and yellow passion fruit juice after high hydrostatic pressure treatment, respectively, by quantitative descriptive analysis (QDA).[13,14] Most volatile compounds have corresponding odor description (Table 1), which are closely related to the aroma descriptions of fruits and vegetables. Through sensory evaluation of fruits and vegetables, we could roughly infer the aroma compounds they contained. Such as sweet, flora and fruity odor is related to esters, green grassy odor is related to hexanal and (*E*)-2-hexenal.[16] Kim et al.[23] analyzed the relationship between GC-MS analysis and human sensory perception of omija. The omija have the ginger, sour aromatics, pine needle, wet grassy and earthy odor, meanwhile, acetic acid and α-pinene in omija is related with sour aromatics and pine, respectively. Du et al. found furaneol, linalool, geraniol, ethyl hexanaote, trans-2-hexenol, and β-ionone in blackberries could account for their similarity in fresh fruity, floral, strawberry, and raspberry aroma; while 1-octen-3-ol, myrtenol, eugenol, and α-terpineol in blackberries could account for their vegetal, woody, mouldy, and cooked fruit flavor.[24] The aroma properties of fruits and vegetables are determined by the structural properties of the compounds they contained, and there is a causal relationship between them. Through the method of molecular sensory science, we can reveal which compound causes the characteristic aroma of fruits and vegetables.

Sensory evaluation is also used to compare the sensory differences between different recombination models and original samples in the process of omission tests and recombination experiments. Zhang et al.[25] compared the sensory analysis radar chart of different aroma recombination models and the original clear red raspberry juice, found the grassy, floral and fruity notes had the greater contribution to overall aroma. However, sensory evaluation is a very subjective analysis method, which is affected by age, gender, region, emotion, physical condition, environment and culture.[26] Hence, the data variations were greatly in sensory tests and the repeatability is poor. Therefore, in order to ensure the credibility of the sensory test data, the sensory evaluation panelists needs to be uniformly trained, and the sensory description and sensory evaluation standards for sample aroma should be unified.[27]

Table 1. Odor descriptions of volatile compounds of fruits and vegetables.

Volatile compounds	Odor descriptions	Reference
Alcohols		
(*E*)-2-hexenol	green, fruity	[15]
1-butanol	overall flavor, sweet aroma	[16]
1-hexanol	fresh, green, earthy	[16]
1-octen-3-ol	mushroom	[16]
3-mercaptohexan-1-ol	sulfur and passion fruit	[17]
3-octanol	earthy, mushroom, herbal	[18]
benzyl alcohol	bitter almond-like, fruity	[19]
benzeneethanol	flowery, floral, vegetal, woody	[20]
linalool	citrus-like, flowery	[15]
furaneol	sweet, caramel, candy	[20]
methanethiol	sulfur, gasoline, and garlic	[21]
nonanol	rose-orange	
octanol	jasmine, lemon	[21]
menthol	mint-like	[15]
Aldehydes		
(*E*)-2-heptenal	green, leaf, and fat	[17]
(*E*)-2-octenal	green and leaf	[17]
3-methylbutanal	malty	[16]
benzaldehyde	sweet, fruity, roasted, almond, fragant, burnt sugar	[21]
phenylacetaldehyde	sweet and fruity	[17]
heptanal	green	[21]
hexanal	green, grassy	[22]
furfural	bread, almond, and sweet	[17]
nonanal	fat, citrus, green, fruity	[21]
octanal	fat, citrus, and green	[17]
(*E*)-2-octenal	green and leaf	[17]
pentanal	almond, malt, pungent	[20]
octanal	green, fruity, orange, citrus	[20]
vanillin	vanilla-like, sweet	[15]
decanal	sweet, aldehydic, waxy	[18]
nonanal	waxy, aldehydic, rose	[18]
Acids		
propanoic acid	sour-like, sweaty	[15]
acetic acid	sour	[17]
hexanoic acid	sweaty, sour, cheesy	[20]
butyric acid	sour and stink	[21]
decanoic acid	soapy, musty	[15]
Volatile compounds	**Odor descriptions**	**Reference**
nonanoic acid	moldy, pungent	[15]
Esters		
ethyl 2-methylbutanoate	fruity	[20]
γ-octalactone	sweet, coconut, and peach	[17]
γ-hexalactone	sweet, spicy, coconut, and hay	[17]
methyl benzoate	herbal, fruity	[22]
Ethyl benzoate	fruity, flower	[22]
ethyl propanoate	fruity, strawberry	[20]
Pentyl acetate	fruity, banana	[16]
butyrolactone	sweet, flowery	[15]
butyl butanoate	rotten apple	[16]
hexyl butanoate	green	[15]
methyl butanoate	fruity, sweet (lulo-like)	[22]
ethyl butanoate	fruity	[20]
ethyl heptanoate	fruity	[17]
ethyl heptanoate	fruity	[17]
methyl hexanoate	fruity, sweet (pineapple-like)	[22]
ethyl hexanoate	fruity and wine	[17]
ethyl octanoate	fat	[17]
3-mercapohexyl acetate	sulfur, grapefruit, and fruity	[17]
butyl acetate	sweets, fruity	[16]
ethyl acetate	ethereal, fruity, sweet	[18]
ethyl isobutanoate	fruity	[20]

(*Continued*)

Table 1. (Continued).

Volatile compounds	Odor descriptions	Reference
Alcohols		
Ketones		
2,3-butanedione	butter	[17]
2,3-pentanedione	butter	[17]
2-heptanone	fruity, sweet, herbal	[18]
3-hydroxy-2-butanone	butter	[17]
β-damascenone	sweety and floral	[16]
β-ionone	flowery, violet-like	[15]
acetophenone	musty and almond	[17]
nootkatone	fruity	[20]
carvone	minty, licorice	[18]
Pyrazines		
2,3,5-trimethylpyrazine	roast and musty	[17]
2-methoxy-3,5-dimethylpyrazine	roast and musty	[17]
2,5-dimethylpyrazine	nutty and roasted	[17]
2-methylpyrazine	roast	[17]
2,6-dimethylpyrazine	nutty and roasted	[15]
Others		
α-pinene	pine, plant	[17]
Volatile compounds	**Odor descriptions**	**Reference**
D-Limonene	citrus-like	[16]
α-terpinolene	fruity, green	[20]
valencene	citrus-like	[20]
dimethyl sulfide	cabbage, sulfur, and corn	[17]
difurfuryl sulfide	roasted	[17]
2-acetylfuran	sweet, almonds, and roasted	[17]
2-ethylfuran	rubbery, pungent, sweet	[20]
benzothiazole	sulfury, rubbery, vegetable	[18]

Through the combination of sensory perception and objective instrumental analysis, it could evaluate aroma characteristics more scientifically and effectively and better explain the relationship between aroma components and sensory experience.

Instrumental evaluation of aroma and application

Instrumental analysis is the main method for qualitative and quantitative analysis of volatile components. The composition of volatile substances in fruits and vegetables is complex; hence, the precondition for identification of aroma is volatile compounds could be separated effectively (Table 2).

Gas chromatography-mass spectrometry (GC-MS)

MS is a powerful structural analysis tool, which could provide more information for structural characterization, and is an ideal chromatographic detector.[28] It can detect all compounds that be ionized, and obtain mass spectrum at each time point which will provide information of molecular structure of compounds and can be used for qualitative and quantitative analysis.[29]

Since the late 1950s, GC-MS has been widely used as a hyphenated technology that can be used to qualitatively and quantify aroma substances. GC-MS qualitatively analyzes volatile compounds by matching the standard spectrum library, and quantifies the extracted analytes at a certain optimal temperature.[29] At present, GC-MS has been the most widely used technology in the analysis of fruits and vegetables flavor, which combines the effective separation ability of gas chromatography on flavor substances and the precise qualitative ability of mass spectrometer on the separated purified substances, so as to achieve the qualitative and quantitative analysis of multi-component substances.[28] It has the characteristics of high separation efficiency, strong identification ability and high sensitivity.[29]

Table 2. Molecular sensory science related technology and method.

Technology and method		Description	Reference
GC-MS		Quality and quantify volatile compounds. It has the characteristics of high separation efficiency, strong identification ability and high sensitivity.	[29]
GC-IMS		The obtained retention time and migration time could accurately characterize the analyte, and the analyte could be quantitatively analyzed through the intensity of the ion signal peak in the ion mobility spectrum; it provides rapid analysis, high sensitivity and variable volume injection, without pretreatment.	[36]
GC×GC-MS		The advantage is that fragments with the same m/z could be further screened through the reaction, with higher selectivity. It has the characteristics of high sensitivity and strong anti-interference ability.	[47]
GC-O	AEDA	Gradually diluted the aroma extracts until evaluators cannot smell it.	[65]
	DF	Multiple members (≥3) are required to evaluate the same undiluted aroma extracts; the operation is simple, time-saving and the sensory evaluators do not need to be strictly trained.	[65]
	OSME	Real-time recording of changes in the odor intensity and odor characteristics of the sample by the evaluator; the requirements for the evaluator are strict, requiring long-term professional training.	[68]
OAV		Evaluate the contribution of aroma compounds in the presentation of aroma characteristics in food substrates.	[61]
Omission analysis		After reconstitution, the specific aroma compounds are removed again to evaluate the effect of eliminating compounds on the overall flavor.	[60]
Aroma reconstitution		All potential active aroma components of the food are in the original concentration in the simulated matrix; the reconstructed aroma model is compared with the original one, and the result is represented by the radar chart.	[60]

GC-MS: Gas chromatography-mass spectrometry; GC-O: Gas chromatography-olfactometry; GC-IMS: Gas chromatography-ion mobility spectroscopy; GC×GC: Two-dimensional gas chromatography; AEDA: Aroma extract dilution analysis; DF: Detection frequency; OSME: Direct intensity method; OAV: Odor activity value.

Generally, GC-MS is mainly applied to establish the volatile fingerprint and determine the aroma contents of fruits and vegetables. The qualitative identification of aroma compounds generally uses database search, standard products and retention index methods. The quantitative methods of aroma compounds mainly include area normalization method, internal standard method and external standard method.

The area normalization method is more convenient; it is often used to compare the content of samples, and does not pay attention to the specific value of the content. Such as, Dou et al.[30] used GC-MS combined with area normalization method evaluated the aroma quality of banana during different harvest time. The external standard method is often used to determine the specific content of volatile compounds in sample, which is also necessary in molecular sensory science. Zhang et al. applied GC-MS combined MS library, standard products, retention index and external standard methods for 3-(methylthio) propanal, 1-octen-3-one and pyrazines identification in dried mushroom.[31] Internal standard method is most widely applied. Chigwedere et al. used this quantitative method to characterize the changes in the fingerprints of the flavor compounds of the beans during the cooking process.[32] Volatile compounds in Chinese jujubes after different treatments was also effectively analyzed by internal standard method.[33]

Gas chromatography- ion mobility spectroscopy (GC-IMS)

Ion mobility spectroscopy (IMS) is an advanced technique for analyzing volatile and semi-volatile compounds.[34] IMS has a fast response and high sensitivity at normal pressure to separate ions according to their mobility in an electric field. In 1972, the first GC-IMS technology was reported. This instrument includes an automatic headspace injector, which could analyze volatiles without any sample pretreatment.[35] The analytes are pre-separated by GC, the concentration of the analytes is controlled and the impurities are separated, and then the ion mobility spectrum is re-separated to achieve a secondary separation.[36] The obtained retention time and migration time could accurately characterize the analyte in two dimensions, and the analyte could be quantitatively analyzed through the intensity of the ion signal peak in the ion mobility spectrum. After processing the data by the software, fingerprints of trace volatile organic compounds can be quickly obtained[,37,][38] However, the IMS library information of volatile compounds is not complete, is still a problem to be solved. Moreover, the quantification of GC-IMS is complicated. The ratio of the maximum signal intensity of the sample to be tested at different concentrations to the ion signal intensity of the initial reaction reagent is used to obtain the proportional coefficient of the sample to be tested at different concentrations.[39] Therefore, GC-IMS is rarely used for qualitative and quantitative analysis of volatile compounds. But because of its spectral data could effectively distinguish different varieties of samples, and could directly reflect the difference in volatile profile. Therefore, GC-IMS is often applied for fruit and vegetable flavor identification, classification and difference analysis.

Li et al. characterized volatile fingerprints of raspberry wines by GC–IMS without chemometric processing, and observed significant differences between different alcoholic fermentation modes.[40] Also, GC-IMS was applied to analyze the fingerprints of the volatile components of different dried mushrooms. The results show that GC-IMS has potential application value in constructing volatile substance fingerprints and volatile component database of *Lentinula edodes*.[41] Li et al. used GC-IMS to determine the volatile components of *Annona squamosa* L. under different storage conditions.[42] 1-MCP was the better treatment for *Annona squamosa* L., this method provided a theoretical basis for storage and preservation of *Annona squamosa* L. Also GC-IMS was applied to monitor the content variations in volatile component in jujube fruits during the blacking process.[43] The characterization of volatiles of lychee wine fermentation using HS-SPME-GC-MS and GC-IMS were done to regulate processing. Results indicated that citronellol was a monomer in lychee. The work provides important new information on aroma development during fermentation.[44]

GC×GC-MS and GC×GC-TOFMS

Because of the different types and quantities of volatile substances in fruits and vegetables, one-dimensional gas chromatography analysis might cause the problem of component co-elution in subsequent mass spectrometry analysis, which might easily cause the loss of key flavor compounds, thereby affecting subsequent component identification accuracy.[45] Therefore, one-dimensional gas chromatography has certain limitations in the analysis of complex samples, the selection of chromatographic columns and the peak capacity of the analytical system.

Therefore, GC×GC obtained more and more popularity in aroma analysis. The principle of GC×GC is to connect two chromatographic columns with different polarities in series. After the sample is vaporized, the components to be tested are separated by the first-dimensional chromatographic column, and then collected and released by the modulator. In the form of pulse, it enters the second-dimension chromatographic column with different polarities and separates again. The two-dimension chromatographic columns are separated according to polarity or boiling point. Finally, the separated components enter the detector and obtain the detection signal.[46] It has the advantages of rapid analysis, large peak capacity, high sensitivity and high resolution, and it could separate and identify complex samples. Also, it could make up for the disadvantages of low resolution, small peak capacity and inaccurate qualitative determination when GC separating complex samples.[47] The combination of GC×GC, with MS and time-of-flight mass spectrometry (TOFMS) could be applied for untargeted and targeted analysis in aroma, and they are significant powerful analytical tools, have a broad prospect of volatile identification application.

Recently, this technique has been applied to the analysis of aroma of foodstuffs such as wine,[48,49] seafood,[50] bread,[51] chocolate[52] and tea,[53–55] Aith Barbará et al. used GC×GC/TOFMS and GC-MS to analyze wine aroma, GC×GC/TOFMS proved to be efficient for solving cases of co-elutions of important wine aroma compounds.[56] Otherwise, there are published studies describing the use of two-dimensional instruments in the field of banana *Terra* spirit aroma research.[57] In this study, Capobiango et al. found 3-methylbutan-1-ol, 3-methylbutan-1-ol acetate, 2-phenylethyl acetate and phenylethyl alcohol were principal volatile compounds in banana *Terra* spirit.

Gas chromatography-olfactometry (GC-O)

Early research on the flavor of fruits and vegetables was limited to detecting and analyzing a large number of volatile compounds, and searching compounds with corresponding sensory attributes based on the odor characteristics of fruits and vegetables. However, with the development of science and technology, the number of identified volatile compounds continues to increase. So far, thousands of volatile compounds have been found in fruits and vegetables, and it is very difficult to verify the sensory characteristics of these volatile compounds one by one. And although some compounds have a high content and easy to be detected by instruments, because of their high aroma threshold, their contribution to the flavor of fruits and vegetables is limited; and some aroma components with important sensory contributions are difficult to be detected by instruments due to their low content. In order to solve this problem, GC-O technology came into being.[58]

Different from the traditional chemical analysis, the core idea of GC-O is to combine instrumental analysis and sensory analysis, so as to realize the change from chemical composition analysis to flavor composition analysis.[59] GC-O associates the human nose as a detector with GC or GC-MS. It could identify key aroma compounds that affect aroma of the entire food and determine the aroma intensity of odorous substances.[60] The commonly used detection technology in GC-O can be roughly divided into the following 3 types according to different principles which was shown in Fig. 1.

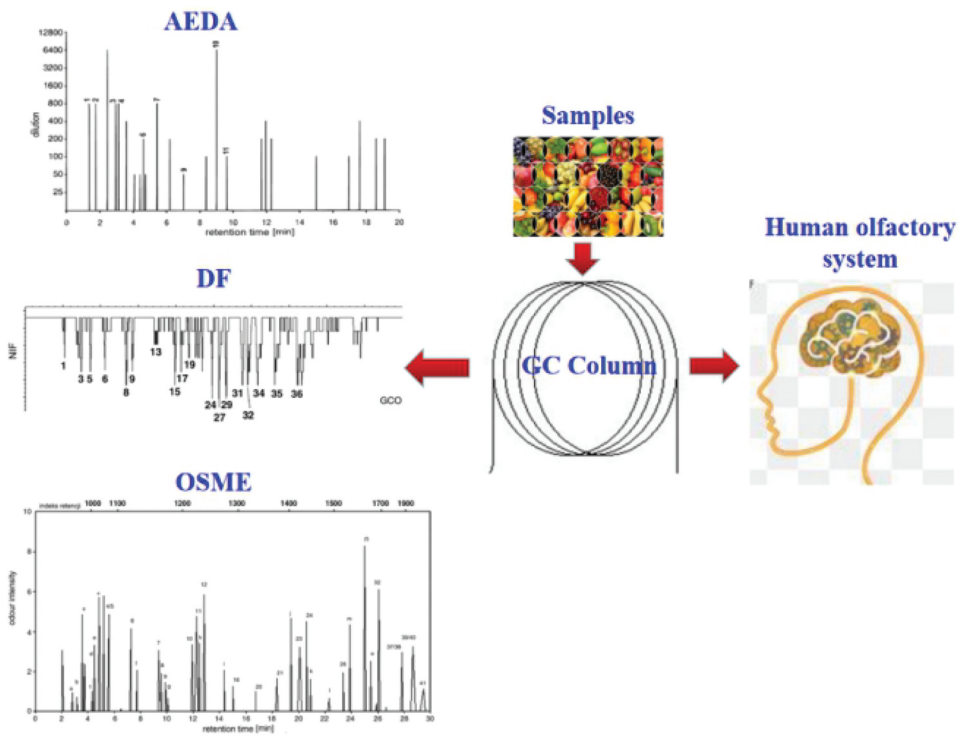

Figure 1. Three types diagram of GC-O tests. AEDA, aroma extract dilution analysis; DF, detection frequency; OSME, direct intensity analysis. Reproduced from Plutowska and Wardencki.[58].

Aroma extract dilution analysis (AEDA)

The dilution to threshold method is a relatively widely used GC-O method. In this method, aroma compounds are gradually diluted. Each diluted concentration sample is subjected to GC-O analysis and sensory evaluation. The group members (usually 8–12) record the retention time, intensity value, and aroma descriptor in the sniffing mouth. The most commonly used methods for dilution to the threshold are AEDA and charm analysis.[61] In charm analysis, panelists evaluate samples with a random order of dilutions. Then, the panelists would record the duration of each detected odor, the results were shown by aroma graph which was generated by plotting the duration of the odor sensation against the dilution value. While, in AEDA, panelists evaluate samples with increasing dilution order and the contribution of an odor active compound is given by its dilution factor (FD) value. The overall results were reported by listing the FD values.[62] Amanpour et al.[62] used GC-O technology to study the main components of fresh and roasted *P. terebinthus* fruits, and the odor active ingredients in fresh and roasted samples were obtained by AEDA method. Pinocarvone and dodecanoic acid were detected only in fresh fruits, while pyrazine class, 5-methylfurfural and γ-butyrolactone were emerged only in roasted fruits. Liu et al.[63] studied the volatile substances in different watermelon juice. Through the GC-O dilution method, 55 odor active substances were obtained. Among them, found the (*Z*)-6-nonenal, (*E, Z*)-2,6-nonadienal, (*E*)-2-nonenal, and (*E, E*)-2,4-nonadienal contributed greater to aroma profiles than alcohols due to lower threshold through odor active values. Similarly, Sonmezdag et al. elucidated the aroma-active compounds of flower buds of both fresh and fermented caper using aroma extract dilution analysis and GC-MS-olfactometry. They found that methyl isothiocyanate in fresh caper and acetic acid in the fermented caper had the highest flavour dilution factor.[64]

However, the dilution method also has its own contradictions and drawbacks. For example, if there are more evaluators performing the evaluation, the analysis time would be longer. However, fewer evaluators would reduce the accuracy and reliability of test results. In addition, the test results depend on the threshold properties of the volatile compounds themselves, rather than the realistic intensity of the analyte odor in a given sample.[58]

Detection frequency analysis (DFA)

In the DFA fragrance spectrum, the peak height indicates the number of times it is smelled, and has nothing to do with the intensity of the fragrance. There are two common frequency detection methods. One is to characterize the fragrance contribution of each substance by the total number of times that each substance is smelled by the scent staff. In the test, substances with a DF≥2 and at least one smell by each of the three evaluators were determined as the odor active compounds of the test raw materials.[65] The other method is characterized the contribution of these substances to the aroma by the size of the Nasal impact frequency (NIF). This method has been applied in the identification of key aroma components in some fruits and vegetables. Lignou et al.[66] studied the flavor substances in different varieties of melon systematically. According to the intensity method of GC-O, it was found that the key aroma components in melon were composed of 15 esters compounds. Kraujalyte et al.[67] studied the odor active substances of fruits juice by DF method. The aroma contribution substances with NIF value≥80% mainly include ethyl 2-methylbutyrate (fruity) and ethyl 3-methylbutyrate (fruity), nonanal (grass), ethyl decanoate (fruity, sweet), methyl butyrate (sweet and apple), ethyl hexanoate (fruity), etc.

But DF also has certain limitations and the results are only related to whether the evaluators could perceive volatile compounds, and furthermore, the results are related to the threshold of volatile compounds. If the concentration of each volatile compound in the analyte is higher than its detection threshold, they would always be detected by the evaluators, so the same DF value would be obtained. However, this result could not reflect the aroma intensity of the volatile compounds and their contribution to the overall aroma.[65]

Direct intensity analysis

The direct intensity method, also called OSME (odor) method, uses a computerized 16-point system to record the change in odor intensity over time and the corresponding odor characteristics, and obtains an OSME spectrum similar to FID detection.[68] In the OSME spectrum, the peak of the spectrum is higher, the odor intensity of the compound and its contribution to the fragrance are greater. This method has relatively few application for the evaluation of key aromas due to the high requirements for the evaluators and the long-term smell training required for the evaluators.[68] Kang et al.[69] identified the aroma active substances in myricarubra using GC-O and GC-MS techniques. It was concluded that the important aroma compounds in myricarubra were mainly caryophyllene, menthol, linalool, phenethyl alcohol, acetic acid by the intensity method and other substances.

These three GC-O methods have their own advantages and disadvantages. In general, AEDA takes the longest time and requires systematic training of evaluators; similarly, OSME also has higher requirements for evaluators; DFA method is the simplest method and the easiest to operate and does not require evaluators to train, but not so accurate in some cases. Therefore, these GC-O methods could be used at the same time to complement each other to obtain accurate and reliable results.

Odor activity value (OAV)

OAV could explain which compounds revealed by GC-O actually contribute to a specific aroma. By accurately quantifying the compound, and then calculating the OAV based on the aroma threshold of the compound in the corresponding matrix, the contribution of the compound to the characteristic odor of the food could be judged. When the OAV value is greater than 1, it indicates that the compound has an aroma contribution in the corresponding food system. And the OAV value greater, its contribution is greater.[61] Furthermore, all the compounds with aroma contribution are added to the corresponding simulation matrix according to the quantitative results, and the aroma model is reconstituted to determine the accuracy of the quantitative results. Finally, the omission test is used to judge the influence of a certain aroma compound or a type of aroma compound on the target characteristic odor, so as to further identify the key characteristic odor compound.

This method has been successfully applied to the identification of key aroma substances in fruits, vegetables and their products such as apple juice,[16] *terebinth* fruits,[70] and mushroom.[18] In order to explore the consistency of the analysis results of different key aroma identification methods. Zhang et al.[71] used OAV and DFA GC-O to identify the odor active components in mango juice. The results showed that a total of 42 volatile substances were identified in mango juice, and 6 components were detected only by OAV, while 4 components were detected only by DFA. The two methods are consistent in identifying key aroma components of mango juice, and each has its own characteristics. The OAV method simplifies the analysis of complex aromas in food.

Zhang et al.[19] identified the odor active compounds of raw and dry porcini mushroom (*Boletus edulis*) by GC-MS, GC-O and AEDA. The selected aroma compounds were quantified and OAV were calculated, indicating that the OAV of 12 compounds in raw porcini were ≥1, and 1-octen-3-one had the highest OAV value. In addition to compounds with eight carbon atoms, 3-methylbutyraldehyde, (*E,E*)-2,4-decadienal and (*E,E*)-2,4-nonadienal also present unique aroma. In dried porcini mushrooms, 20 compounds with OAV ≥ 1 were obtained. Among them, 3-(methylthio) propionaldehyde, 1-octene-3-one and pyrazine were identified as the predominant odors. Zhang et al. analyzed the odor active compounds in red raspberry juice and identified 31 odor active compounds (OAV≥1). Three C6 aldehydes had the highest detection frequency (8) using GC-O. And the characteristics flavor of red raspberry juice was mainly described as floral, herbaceous and woody.[25]

In 2019, An et al.[72] used the concept of molecular sensory science to characterize the cooked off-flavor in heat-sterilized lychee juice (HLJ). Fifteen kinds of compounds with increased OAV value in the HLJ was identified via GC-O-AEDA test and OAV calculation. Finally, it was confirmed through recombination and omission tests that DMS, methionine, DMTS, DMDS, 3-methylbutyraldehyde and 2,4-dithiapentane had a significant negative effect on the overall aroma of HLJ. The research first adopted the research ideas of molecular sensory science to determine the compounds related to the characteristics of cooked odor, and then determined the key cooked odor signature markers through the analysis of multiple samples.

Conclusions and Future Perspectives

Research of the aroma of fruits and vegetables have been advanced in recent years, more sensory-related compounds in fruits and vegetables could be identified and applied to the final products. As indicated here, increased future use of molecular sensory science technology could provide us valuable new exploration methods. This review illustrated the analysis techniques related to molecular sensory science. GC-MS, GC×GC-MS and GC-IMS would be used to qualify and quantity the volatile compounds. When they are used in combination with GC-O, OAV, omission test and reconstitution experiment, this allows us not only to identify sensory-related compounds, but also to screen out key aroma compounds from many volatile compounds.

However, molecular sensory science technology also has certain limitations. The matrix of fruits and vegetables is complex. Some fruits and vegetables that contain more polysaccharides interact with volatile compounds, and there are also certain interactions between volatile components. In the application of molecular sensory science technology, these interactions were ignored, resulting in the inability to accurately reproduce the odor characteristics of fruits and vegetables. Therefore, it is necessary to systematically understand the odor binding characteristics of these components, and develop systematic research on the interaction between fruit and vegetable matrix and volatile components.

At present, GC-O-MS is the most widely used in molecular sensory science technology, but the volatile substances in fruits and vegetables have different types and quantities. One dimensional chromatographic separation analysis might cause the problem of co-elution of components in subsequent mass spectrometry analysis, which is likely to cause volatile flavor analysis. The loss of key aroma compounds in the medium, thereby affecting the accuracy of subsequent component identification. Therefore, how to ensure better separation and more precise certainty of volatile mixtures is another technical difficulty in flavor research. Newly developed multi-dimensional chromatographic separation technologies provide a good solution for the separation of complex mixtures. In the future, these technologies such as GC×GC-MS could be combined with olfactometry to provide more accurate and diverse flavor analysis methods.

Sensory evaluation is also an important step in molecular sensory science technology. However, sometimes inaccurate results were obtained in the sensory evaluation because of the different sensitivity of sensory evaluators. Therefore, it is necessary to strengthen the professional training of evaluators, establish a complete evaluation system, try to avoid human errors, and ensure the objectivity and consistency of the evaluation results. In addition, olfactory visualization analysis technology, bionic olfactory technology fused with intelligent detection, etc., combined sensory analysis with intelligent instruments, which could replace traditional sensory evaluators, reduce the training time of evaluators and make experiment results more objective.

At present, molecular sensory science technology is mainly used to describe the sensory properties of fruit and vegetable aroma and explore the volatile compounds that cause different sensory characteristics of fruits and vegetables. However, there are few studies on flavor quality control of fruits and vegetables and their products, consumer preferences research on flavor and development and application of flavor products. Therefore, the continuous promotion of the application of molecular sensory science technology in the flavor of fruits and vegetables and their products could further accelerate the development of the fruit and vegetable processing industry and explore fruit and vegetable products that consumers like.

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