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Application News

GC-MS GCMS-TQ™ 8040 NX

Vegetable Juice Evaluation by Particle Analyzer and GC/MS

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User Benefits

- The Smart Aroma Database™ helps detect low-concentration aroma components in MRM mode.
- The Multi-Omics Analysis Package can detect particle size concentrations and sizes contributing to differences between samples, using both primary metabolite and particle measurement data.

■ Introduction

In recent years, the demand for vegetable juices has increased with the rise of health awareness. As more people demand a health-conscious diet, vegetable juices are popular because they are nutrient-rich and easy to consume. However, there are a variety of vegetable juices on the market, and consumer tastes are diversifying. For example, there are various kinds of vegetable juices, such as vegetables that combine tomatoes, cabbage, and carrots, and smoothies that combine fruits and vegetables. Therefore, in developing vegetable juices, it is necessary to provide products tailored to consumers' tastes and needs.

Analyzing particle size and aroma concentration is crucial in developing vegetable juices. Large grain size can affect palatability and ease of drinking, while inappropriate aroma concentration can lead to an unattractive flavor.

Quality and taste of vegetables may vary due to seasonal changes, cultivation methods, soil and climate conditions. This presents a challenge for product developers who require an objective evaluation method.

This application presents an example of measuring 4 types of commercially available vegetable juices using the dynamic particle image analysis system iSpect DIA-10 and the gas chromatograph mass spectrometer GCMS-TQ™ 8040 NX equipped with AOC-6000Plus (Fig. 1). Particle size distribution was measured using a 300 µm cell (special type) to evaluate particle concentration and shape. GC/MS measured 484 aroma components using the Smart Aroma Database. The results were integrated and analyzed using the Multi-Omics Analysis Package (Garuda).

Fig. 1 iSpect DIA-10 (left) and GCMS-TQ™ 8040 NX (right)

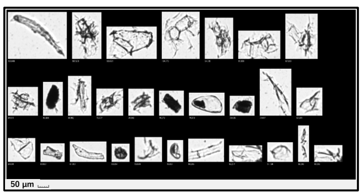
■ Experimental

Particle size distribution was measured by diluting 4 kinds of commercial vegetable juices 100 times and 500 times with pure water. For GC/MS measurements, 200 µL of commercial vegetable juice stock solution was sealed in a 20 mL headspace vial. Measurements were performed per the Smart Aroma Database.

Fig. 2 Four Commercial Vegetable Juices

■ Integrated analysis of particle concentration and aroma components

In the particle concentration measurement, the particle concentration of the undiluted solution was calculated from the measurement results of 100 times dilution rate for the samples A and B and 500 times dilution rate for the samples C and D. The particle concentration of sample A was 170 particles/mL and that of sample C was 1520 particles/mL (Fig. 3). Sample A also had the lowest median diameter. Humans can feel roughness on the tongue even when the particle size is about 10 µm, and it was assumed that roughness would be felt in all samples measured in this time[1].



sample	Particle concentration (count/mL)				
	Total	20-50 µm	50-100 µm	100-250 µm	250-500 µm
A	170	168	2	0	0
B	546	464	51	24	7
C	1520	1333	139	49	0
D	1299	1140	108	46	4

Fig. 3 Particle images (left) and concentration (right)

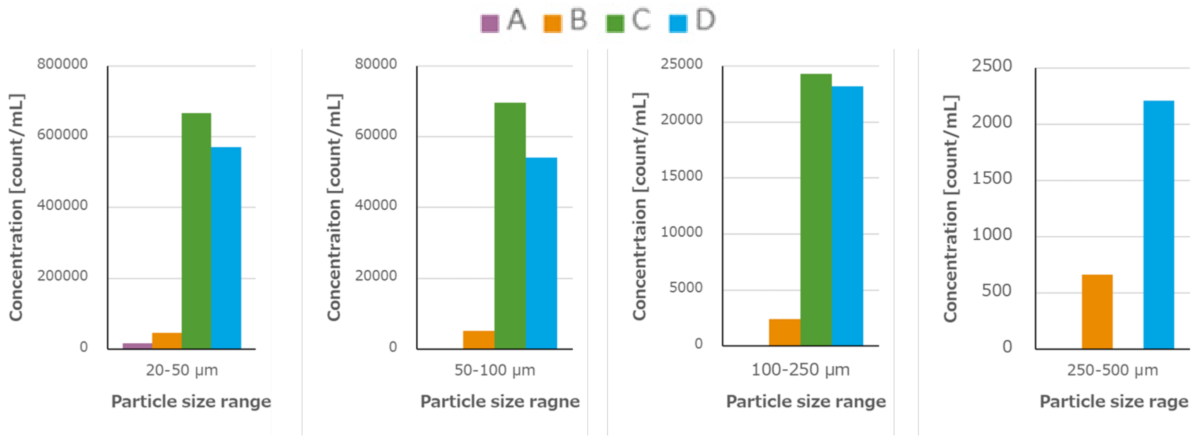


Fig. 4 Particle concentration (equivalent to those in undiluted juice)

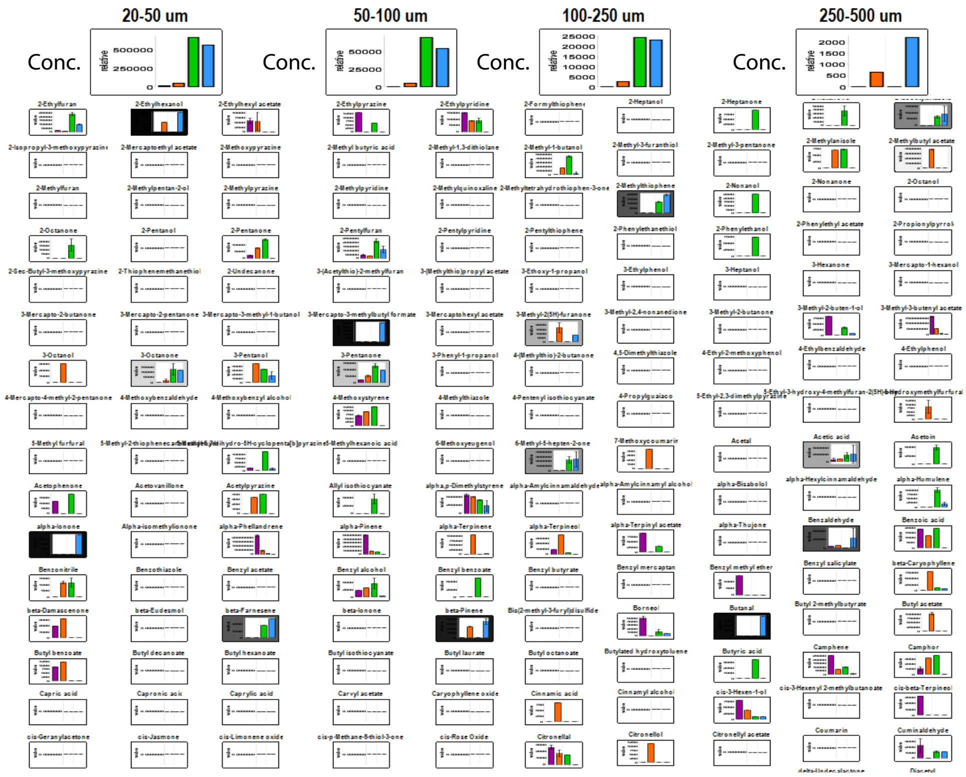


Fig. 5 Visualization of correlation between aroma components and particle size (search for aroma components similar to 250-500 µm)
*The darker the background color of each compound, the higher the positive correlation.

The concentration and size of vegetable particles vary depending on the crushing method used to prepare the juice, the temperature at which it is pureed, and the mesh size. Thus, the size and shape of the particles produce different particle sensations in the mouth. However, the effect of taste and flavor on the perception of particle sensation has yet to be studied.

Therefore, we measured the correlation between aroma components and particle size. GC/MS measured 484 flavor components, and more than 100 were detected in each sample. The particle size distribution was divided into 4 sections: 20-50 µm, 50-100 µm, 100-250 µm, and 250-500 µm (Fig. 4). The calculated concentration distribution was visualized as a bar graph, and correlation analysis was performed with aroma components using the map function of the Multi-Omics Analysis Package (Fig. 5). The results showed that large particle size was highly correlated with 2-ethylhexanol (rubbery odor), β-pinene (forest odor), and propyl acetate (pear odor). Small particle size correlated with 2-pentylfuran (sweet aroma), geranyl butyrate (fruit aroma), pentyl butyrate (sweet aroma), and 3-octanone (fruit odor) (Fig. 6).

By identifying these correlated compounds, it is possible to add them (e.g., β-pinene, which is correlated with larger particle size, to juices with smaller particle size) and conduct sensory evaluations to plan research on the effects of flavor on particle sensation perception (e.g., enhancing or masking the sensation of roughness).

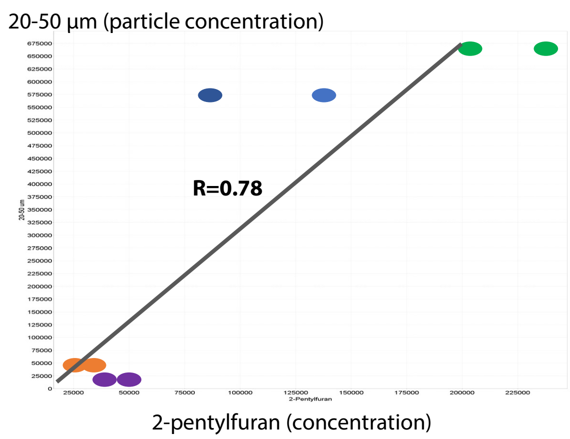


Fig. 6 Correlation between particle size of 20 -50 µm and 2-pentylfuran

By using the Volcano plot to compare samples with smaller particles (A and B) with samples with larger particles (C and D), we detected specific flavor components in each particle size group (Fig. 7).

The juice with small particles contained 11 specific aroma components, including 1-hexanol (unpleasant odor), octanal (fruit odor), and ethyl 2-methylbutyrate (fruit odor). On the other hand, the juice with large particles contained 10 specific aroma components, including 6-methyl -5 heptene -2 -one (citrus odor), 2-ethylfuran (chocolate odor), and 2-butanone (minty odor) (Fig. 8). In addition, some components were found to be common or not present in either sample group (e.g., butter-smelling diacetyl).

■ Statistical analysis of particle shape

The iSpect DIA-10 simultaneously analyzed not only the particle concentration but also the shape of each sample. The shape of each of the 323 particles detected in Sample A was quantified using 31 items, including area based diameter, maximum length, circularity, aspect ratio, ferret diameter, and brightness. The shape of 836 particles of sample B, 2060 particles of sample C, and 1409 particles of sample D were also observed in 31 items. A total of approximately 4500 pieces of particle shape information were loaded into the Multi-Omics Analysis Package and subjected to principal component analysis (Fig. 9 below). As a result, it was found that the area based diameter was specifically low in sample A. It was also found that there was no correlation between the circularity distribution and the sample type (Fig. 10).

Principal component analysis revealed that particle numbers 58 and 72 of sample B were characteristic among the particles of 4 samples. Particle numbers 58 and 72 have a large area based diameter (307 µm, 344 µm) and a pattern width (296 µm, 306 µm), which can greatly affect the texture. It is known that sweet taste components (sugars) reduce the graininess, but the relationship between sweet aroma and graininess needs to be investigated in the future[2].

■ Summary

Four commercially available vegetable juices were measured using a dynamic particle image analysis system iSpect DIA-10 and a gas chromatograph mass spectrometer GCMS-TQ™ 8040 NX with an AOC-6000Plus. In the particle size distribution measurement, 20-500 µm particle size distribution was evaluated using a 300 µm cell (special type). GC/MS measured 484 aroma components using the Smart Aroma Database and detected more than 100 components in each sample. Particle concentration and aroma content measurements were integrated and analyzed using the Multi-Omics Analysis Package (Garuda). It was found that aroma components correlated with particle size could be detected and utilized for quality control and product development of vegetable juices.

<References>

1) Particle Size Analysis for Food & Beverage, Shimadzu Corporation, accessed on Dec 27th, 2023
2) 温度及び味・風味が粒子に関連する口中感覚に及ぼす影響 [Effect of Temperature, Taste, and Flavor on Intraoral Granular Sensations Produced by Particles], Journal of the NARO Research and Development, accessed on Dec 27th, 2023

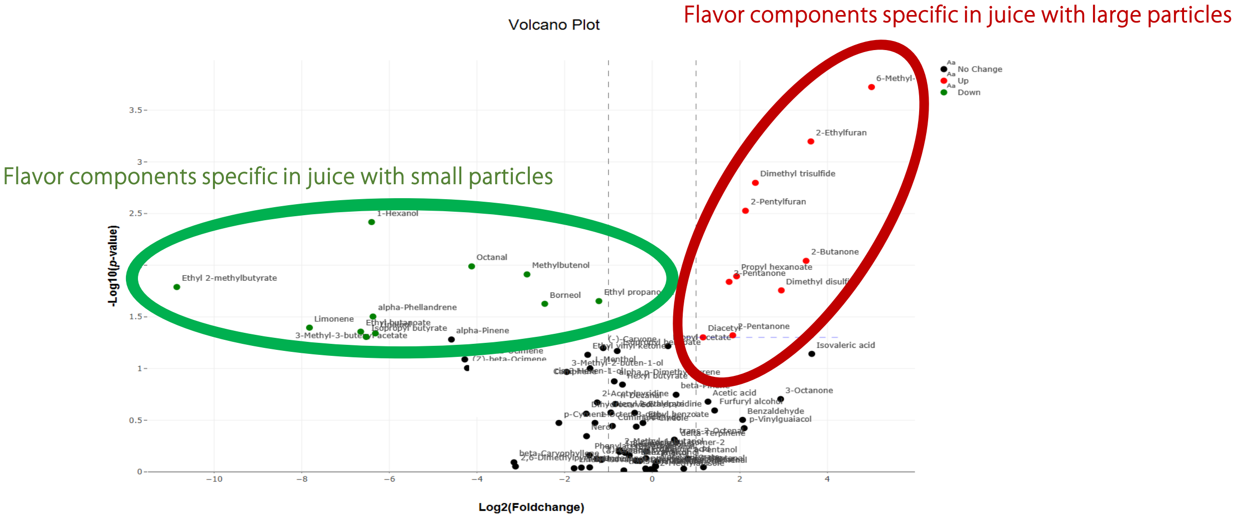


Fig. 7 Volcano plots of samples with small particles (A and B) and samples with large particles (C and D)

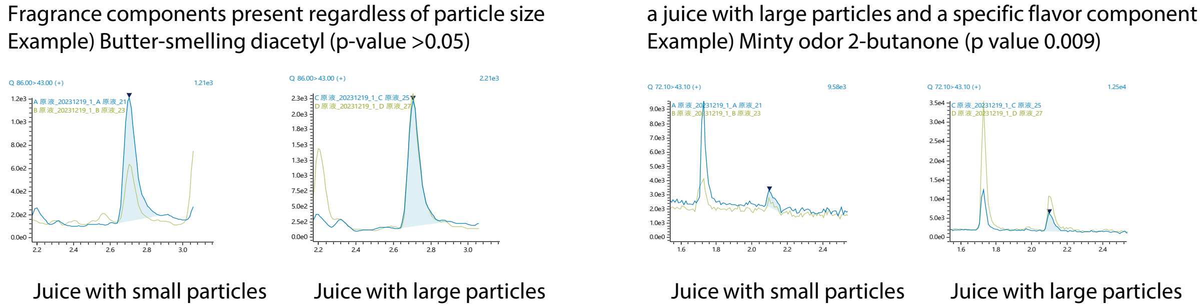


Fig. 8 Example chromatograms of samples with small particles (A and B) and samples with large particles (C and D)
(Overlaid chromatograms of the samples A and B on the left and the samples C and D on the right)

Fig. 9 Visualization of particle shape distribution by principal component analysis

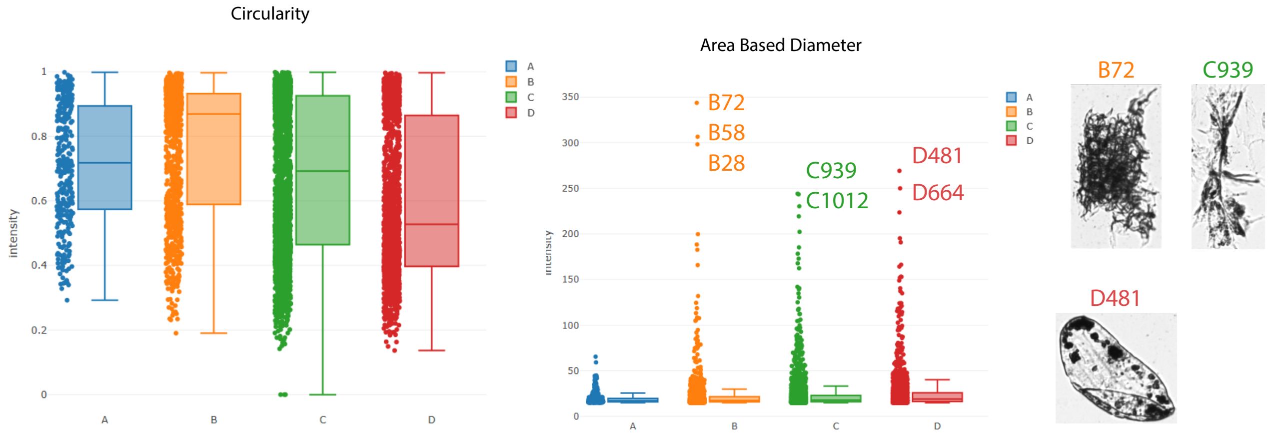


Fig. 10 Visualization of particle shape distribution by box plot
(Left: No difference in circularity; Right: Sample A is low in area based diameter)

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