# Ambient Ionization Mass Spectrometric Detection of Aroma Released During Gummy Chewing

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## 1. Introduction

◆In recent years, there has been growing interest in evaluating flavor using analytical instrumentation, and retronasal aroma during eating is important. In this study, we proposed an analytical method for measuring retronasal aroma during eating using a single quadrupole mass spectrometer (LCMS-2050) equipped with an ambient ion source (Dark Current Discharge Ionization : DCDI) without pretreatment.

Figure 1. Appearance of LCMS-2050 and DCDI

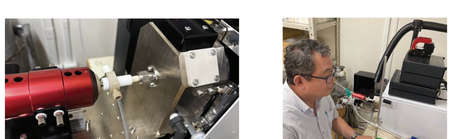


Figure 2. Sample Injection unit (SIU) tube attached to DCDI and a view of the measurement

## 2. Methods

1) The aroma of grape-flavored gummies with different physical properties was measured. Commercially available grape-flavored gummies were used. The types of gummies measured were (a) soft, (b) hard, and (c) soft and elastic. The method for measuring gummi intake is shown in Figure 3. The analysis conditions for DCDI and LCMS are shown in Table 1.

2) The differences in the aroma of food combinations were measured. The differences in the aroma of sake, sashimi, and wasabi were examined. As in Fig. 3, the participants drank sake 60 seconds after the start of measurement and drank it 3 times every 1 minute. The participants ate sashimi 30 seconds after drinking sake.

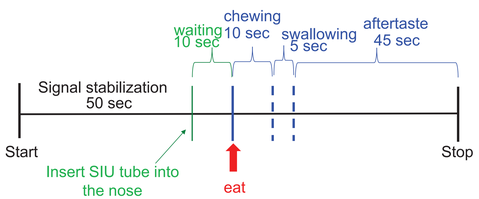



Figure 3. Measurement condition

Table 1. Analytical conditions

| DCDI | | Mass spectrometer | |
|---|---|---|---|
| System | :DCDI | System | :LCMS-2050 |
| Gas heater temp | :OFF | Polarity | :Positive |
| Ar gas flow rate | :0.5 L / min | DL temp. | :200 ℃ |
| $N_2$ gas flow rate | :2.0 L / min | Heat block temp. | :OFF |
| | | Interface Voltage | :+2.0 kV |
| | | Scan range | :*m/z* 40-300 |
| | | Event time | :0.195 sec |

## 3. Results-1

◆The total ion current chromatogram (TICC) of LCMS-2050 was used to compare the aroma profiles of three types of gummies in Figure 4. The three types of gummies differed in how TICC intensity changed from the start of eating.

◆Since the ion intensity detected during eating changes every second, the whole picture can be captured by developing the heat map in Figure 5.

◆The three-dimensional diagram in Figure 6 makes it easier to visually understand and consider the sensory evaluation during eating.

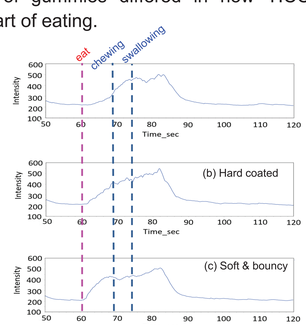



Figure 4. Total ion current chromatogram (TICC)

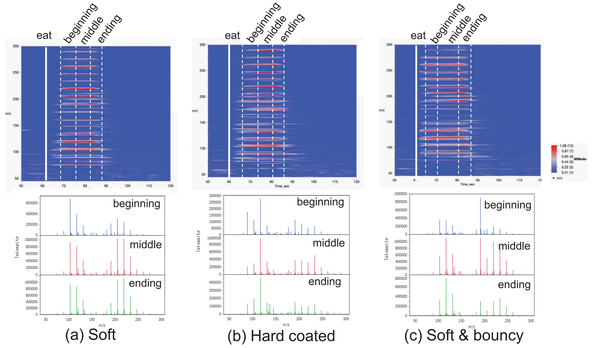
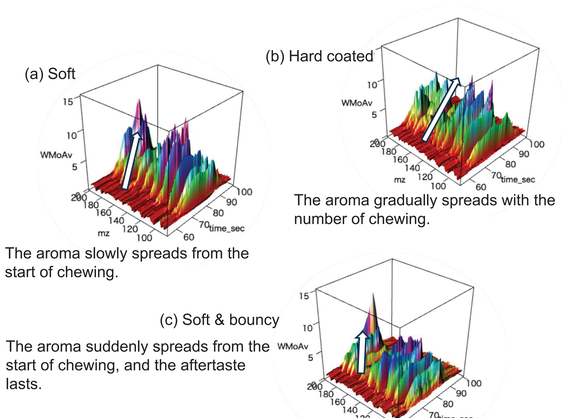



Figure 5. Heat map (upper) and mass spectral changes (lower) in time series during eating




The aroma slowly spreads from the start of chewing.

The aroma gradually spreads with the number of chewing.

The aroma suddenly spreads from the start of chewing, and the aftertaste lasts.

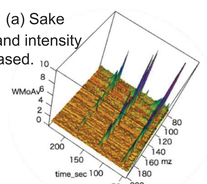
Figure 6. Three-dimensional diagram of mass spectral changes in time series during eating gummy
(drawing using statistical analysis software "R" )

## 4. Results-2

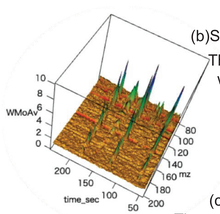
◆Figure 7 shows the results of visualizing the marriage between sake and food. The measured data were subjected to weighted moving average processing to highlight the changes. (Algorithm developed by AMR,Inc.)

Shimadzu Original Japanese sake
"Gen en ryu cho"

(a) Sake
By the third time, the number and intensity of the peaks had decreased.




(b)Sake＋sashimi.
The number and intensity of peaks were high even in the third time.




(c)Sake＋sashimi with wasabi
The number and intensity of peaks were higher even in the third time.

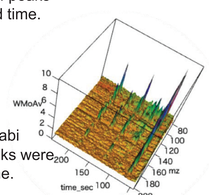



Figure 7. Three-dimensional diagram of mass spectral changes in time series during drinking and eating
(drawing using statistical analysis software "R" )

## 5. Conclusion

◆We developed a simple method for evaluating retronasal aroma using a single quadrupole mass spectrometer with an ambient ionization source. Ambient ionization mass spectrometry (DCDI LCMS-2050) can rapidly measure retronasal aroma during eating. Time-resolved visualization reveals texture-dependent differences in aroma release dynamics among grape-flavored gummies. It is also expected to lead to the visualization of the marriage between food and alcohol. This approach may facilitate objective evaluation of flavor release during consumption and support product formulation and sensory science.