# An Enhancing Device for Volatile Compound Analysis for DART<sup>®</sup>-MS ~ Volatimeship ~

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### Volatimeship

Gas chromatography/mass spectrometry (GC/MS) is typically used for analysis of volatile compounds, such as aromas, flavors, fragrances and outgassed compounds. For qualitative analysis, GC/MS is a powerful analysis method, but due to the time required for GC separation, it is not suitable for continuous monitoring of changes over time.

DART<sup>®</sup>-MS analysis, a direct analysis method, enables near instantaneous determination of sample composition via mass spectrometry. Although DART®-MS also enables determination of volatile compounds, when the samples contain only small amounts of the volatilized target compounds diffusion can make them undetectable in the open environment of the DART®-MS system.

In order to overcome this issue, we developed a closed-chamber interface device called Volatimeship (Fig.1). Volatimeship combined with DART<sup>®</sup>-MS is an effective method to monitor volatile compounds with short analysis times and high sensitivity.



Fig.1 Volatimeship



Fig.2 Volatimeship combined with DART<sup>®</sup>-MS system



### **Application 1**

### **DRIP BREWED COFFEE**

#### INTRODUCTION

Coffee is a brewed drink prepared from roasted coffee beans, which are the seeds of berries from the Coffee plant. It is a favorite beverage which is drunk all over the world. Many people feel relaxed when they smell the aroma of coffee. Therefore, in the field of medicine and beauty, there is ongoing research into the aroma of coffee. The purpose of this application was to detect the aroma at the moment when the coffee was brewed

• **SAMPLE** Drip brewed coffee

#### METHOD

The analysis system was composed of Volatimeship equipped with the DART<sup>®</sup>-MS. 10 mL of coffee was placed in a 40 mL vial, and then the sample vial was sealed. First, a blank vial was attached to the Volatimeship, data acquisition by the mass spectrometer was started, and then the background was measured. After measuring the background, the blank was replaced with a vial containing coffee, and then the volatile compounds were directly measured.

#### RESULT

The total ion current chromatogram is shown in Fig.5(A). The time when a vial contained coffee was attached to Volatimeship was indicated as 0 second. Immediately after attaching the vial containing coffee, the total ion current of volatile compounds volatilized from coffee spiked up. Extracted ion current chromatograms are shown in Fig.5(B). m/z 80 gradually attenuated after an initial spike while m/z 160 gradually increased 6000 Additionally, m/z 123 was released all at once in a short time immediately after attaching the vial containing coffee.

In summary, Volatimeship combined with DART<sup>®</sup>-MS enables detection of the release behavior of volatile compounds from coffee, directly and rapidly. Therefore, it could contribute to further research on aroma in the field of medicine and beauty.











### Application 2

### **BATH ADDITIVES**



#### INTRODUCTION

In Japanese culture it is common to include bath additives when bathing. For example, we add iris during the Boys' Festival and citron during the Winter Solstice. The time spent choosing and dispensing bath additives is pleasant: since a good smell is spread after putting in a bath additive, it makes us forget fatigue.

The purpose of this application was to detect the smell of bath additives at the moment when we put the bath additives into a bath.

• SAMPLES Bath additives (Maker A, Maker B These were the same type of fragrance products.



#### METHOD

The analysis system was composed of Volatimeship equipped with the DART<sup>®</sup>-MS. In addition, a separable flask containing 40°C hot water was connected to Volatimeship, and maintained at a warm temperature (Fig.6). After measuring the background, a bath additive was put into the separable flask, and then the volatile compounds were spread and measured directly.

#### RESULT

Mass spectra taken 30 seconds after inserting the bath additives are shown in Fig.7. Even though both comprised the same kind of fragrant products, detected ion kinds and intensity were different between the two samples. Therefore, it can be applied as a rapid screening method (measurement time: ONLY 1 minute). Additionally, the release behavior of the compounds of each bath additive is shown in Fig.8, in which they were monitored over 60 seconds.

In summary, Volatimeship combined with DART®-MS enables detection of the release behavior of volatile compounds from bath additives, directly and rapidly. Moreover, combining this method and sensory evaluation could be useful for characterizing products during development and contribute to further research in the field of medicine and beauty.





## **Application 3**

### **CITRUS FRUIT**

### INTRODUCTION

The aromas of citrus fruits are widely favored because they help us to relax. "Shonan Gold" is a type of citrus fruit local to the Kanagawa-prefcture of Japan. In our previous investigation, we showed that linalool is part of Shonan Gold's characteristic floral scent. Therefore, we investigated the release behavior of linalool from Shonan Gold.

#### • SAMPLE

Shonan Gold (Citrus fruit)

#### METHOD



The analysis system was composed of Volatimeship equipped with the DART<sup>®</sup>-MS, the MS was a triple quadrupole mass spectrometer LCMS-8030 (Shimadzu Corporation, Kyoto, Japan). In addition, a separable flask containing whole Shonan Gold was connected to Volatimeship (Fig.9). After measuring the background, the Shonan Gold was squeezed, and then the volatile compounds were spread and detected.

#### RESULT

Linalool was detected as Shonan Gold was set into sample flask and the intensity changed immediately after squeezing. Additionally, Terpinene, limonene, and terpineol were also detected (Fig.10). Continuous monitoring clarified that the linalool was volatilizing both before and after squeezing. Since linalool was volatilizing from Shonan Gold continuously, linalool could be a characteristic scent of Shonan Gold. In summary, Volatimeship combined with DART<sup>®</sup>-MS enables continuous detection of flavor and aroma compounds. Therefore this method could be useful for breeding and flavor analysis of fruits.



T. Sagawa, K. Matsumoto, J. Watanabe, C. Takei, M. Sakakura, T. Shiota, H. Matsufuji, 60th ASMS Annual Conference, Poster, ThP005 (2016)