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# Classification and Visualization of Beer Quality Using GC-MS and GC-FID

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伊勢角屋麦酒

# Overview

Despite the same brand and identical brewing techniques, it is widely known that beer taste and quality is not consistent from plant to plant. Therefore, brewers normally check beer quality mainly by sensory test method, and in turn, adjust beer taste in order to reduce these differences as much as possible. In this poster, by metabolomics profiling using GC-MS and GC-FID, we introduce a new approach towards classification and visualization of beer quality to identify how specific components influence taste from plant to plant.

# Introduction

In food science, global metabolite analysis, or 'metabolomics', is increasingly applied to a number of value-added food production areas including food-safety assessment, quality control, food authenticity, origin and processing. GC-MS are widely used for measuring the total amount of metabolites in a sample. Whereas GC-FID might be less utilized in Metabolomics than GC-MS so far. This is because GC-MS is more powerful in peak annotation, and peak annotation is considered necessary for Metabolomics. But GC-FID has a massive feature; low cost, easy to use, and better reputability.

**GC-MS(/MS)**

- Permits comprehensive measurement of several hundred compounds in a single measurement
- Better peak annotation
- First-choice comprehensive measurement

**GC**

- Simple measurement
- Ideal for efficient routine measurement of specific compounds
- Better repeatability
- Low cost

Figure 1 Instrument Features

# Classification and Visualization of Beer Quality Using GC-MS and GC-FID

In order to introduce a new approach towards classification and visualization of beer quality, we tried doing the following two studies.

**Study1: Classification of different brand beers**
Five brand beers were analyzed by GC-FID and GC-MS, and then principal component analysis (PCA) was performed using each GC-FID and GC-MS data. The results of PCA from each GC-FID and GC-MS data were compared. From loading plot of GC-MS data, we can successfully identify how specific components influence this classification.

**Study2: Classification of same brand beers**
The different plant and lot beers in the same brand were analyzed by GC-FID and GC-MS, and then principal component analysis (PCA) was performed using each GC-FID and GC-MS data. The results of PCA from each GC-FID and GC-MS data were compared. From loading plot of GC-MS data, we can successfully identify how specific components influence this classification.

# Methods

## Samples

After metabolites were extracted from beers, they were derivatized. Table 1 shows pretreatment procedure for the sample of GC-MS and GC-FID, and Table 2 shows types of analyzed beer samples.

Table 1 Pretreatment procedure

50μL degassed beers
↓
An internal standard* was added.
↓
Extraction of hydrophilic metabolites.
↓
Drying
↓
Samples were methoximated and trimethylsilylated.

* 2-Isopropylmalic acid (0.5 mg/mL)

Table 2 Types of analyzed beer samples

| Types of beer | Study1 | Study2 |
|---|---|---|
| Lager A | ○ | |
| Pale ale A (Plant: a) | ○ | ○ |
| Pale ale A (Plant: b, Lot: a) | | ○ |
| Pale ale A (Plant: b, Lot: b) | | ○ |
| Pale ale A (Plant: b, Lot: c) | | ○ |
| Pale ale B | ○ | |
| Pale ale C | ○ | |
| IPA A | ○ | |

## Analytical conditions and software

Pretreated beers were analyzed by GC-MS triple quadrupole mass spectrometer and GC-FID. For statistical analysis, SIMCA 15 software (INFOCOM CORPORATION) was used.

Table 3 Analytical condition in GC-MS/MS

| | |
|---|---|
| **GC-MS/MS** | **: GCMS-TQ8040** |
| **Software** | **: Smart Metabolites Database (475 compounds)** |
| **GC conditions** | |
| Column | : DB-5 (30 m × 0.25 mm I.D., 1.00 μm) |
| Carrier Gas | : He |
| Injection Temperature | : 280 °C |
| Control Mode | : Linear velocity (39.0 cm/sec) |
| Injection Method | : Splitless |
| Sampling time | : 1min |
| Oven Temperature | : 100°C (4 min) - 10 °C/min - 320 °C (11 min) |
| **MS conditions** | |
| Ion Source Temperature | : 200 °C |
| Interface Temperature | : 280 °C |
| Tuning Mode | : Standard |
| Measurement Mode | : MRM |
| Loop Time | : 0.25 seconds |
| MRM Transitions | : 950 Transitions |

Table 4 Analytical condition in GC

| | |
|---|---|
| **GC** | **: GC-2030** |
| Column | : SH-Rtx-1 (60 m × 0.32 mm I.D., 1.00 μm) |
| Carrier Gas | : He |
| Injection Temperature | : 280 °C |
| Control Mode | : Linear velocity (25.0 cm/sec) |
| Injection Method | : Split (1:15) |
| Oven Temperature | : 40°C - 4 °C/min - 320 °C (15min) |
| Detector | : FID |
| Detector Temperature | : 330 °C |

# Results

Principal component analyses (PCA) for GC-MS/MS and GC-FID data were performed in the following study 1 and 2.

## Study1: Classification of different brand beers

### Principal component analyses for GC-MS/MS

Figure2 shows Score plot and loading plot from GC-MS/MS data. From Score plot of figure2, we can confirm that five types of beers were successfully classified. Loading plot of figure2 means which compounds are relatively higher concentration among five beers and how specific compounds influence this classification. Table5 shows higher concentration compounds in each beer from loading plot. In IPA A and Pale ale C, a lot of some sugars were remained.

### Principal component analyses for GC-FID

Figure3 shows the score plot from GC-FID data. We can get almost the same score plot as one of GC-MS/MS. This result suggest that GC-FID can also used for classification of beers quality. Whereas, it is difficult how specific compounds influence this classification from only FID data, because qualitative analyses performance on GC-FID is less than GC-MS.

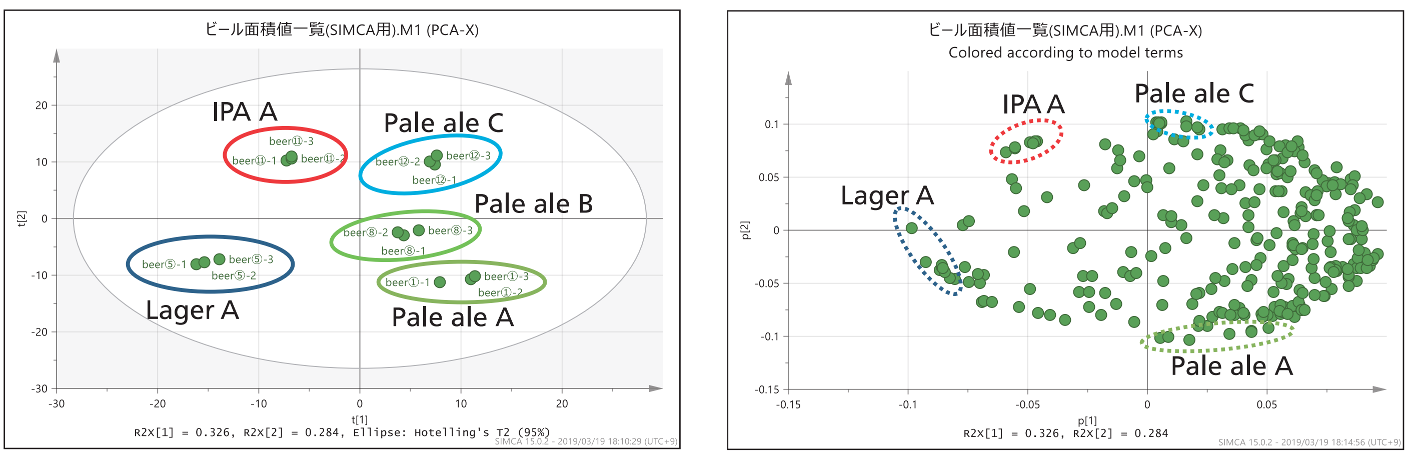


Figure 2 Score plot and loading plot from GC-MS/MS data

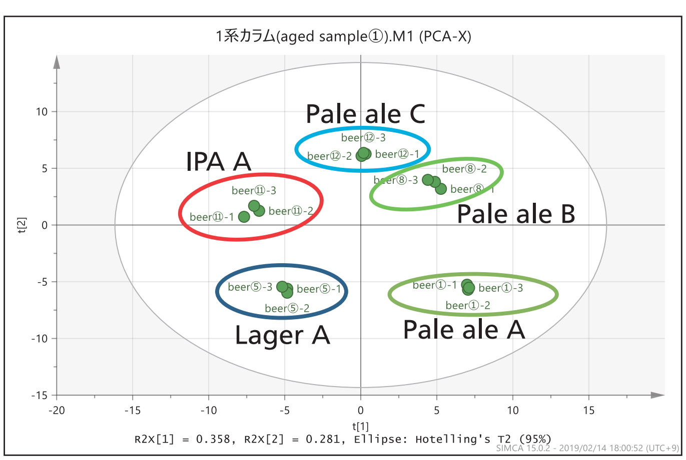


Figure 3 Score plot from GC-FID data

Table 5 Higher concentration compounds in each beer from loading plot

| Types of beer | Higher concentration compounds |
|---|---|
| Lager A | Phenylpyruvic acid, Glutaric acid<br>Lyxose, Xylose, Arabinose<br>Threo-b-hydroxyaspartic acid<br>2-Ketoglutaric acid<br>2-Hydroxyglutaric acid |
| Pale ale A | Maleic acid, Cadaverine, Maltitol<br>4-Aminobutyric acid, Dopamine<br>Tryptophan, Oxalic acid |
| Pale ale C | Galactose, Galacturonic acid<br>Glucose, Mannose, Erythrulose<br>Homogentisic acid, Glucuronic acid<br>Asparagine |
| IPA A | Sebacic acid, Fructose, Sorbose<br>Tagatose, Psicose |

## Study2: Classification of same brand beers

### Principal component analyses for GC-MS/MS

Figure4 shows score plot and loading plot from GC-MS/MS data. From Score plot of figure4, we can confirm that the same brand beers brewed in different plants were divided. Plus, different lots of same plant can successfully classified in the score plot. Loading plot of figure4 means which compounds are relatively higher concentration among the same brand beers and how specific compounds influence this classification. Table6 shows higher concentration compounds in beers brewed in Plant a and b from loading plot. In the beer brewed in Plant a, a lot of metabolites from sugar were remained. These results suggest that this approach could be a powerful tool for adjusting food quality.

### Principal component analyses for GC-FID

Figure4 shows the score plot from GC-FID data. We can get almost the same score plot as one of GC-MS/MS. This result suggests that GC-FID can also used for classification of beers quality in same bland.

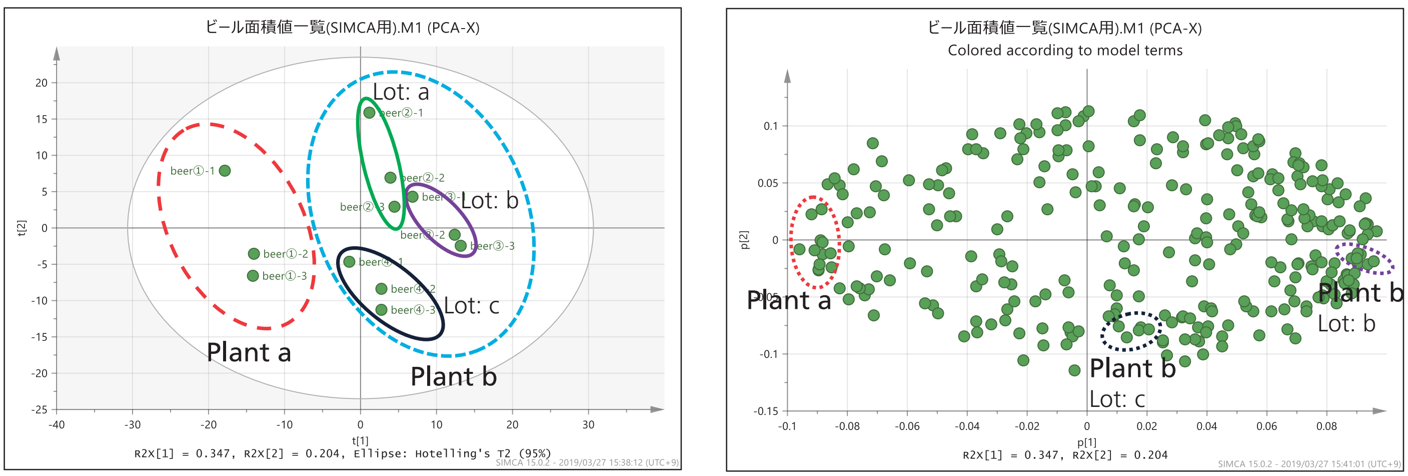


Figure 4 Score plot and loading plot from GC-MS/MS data

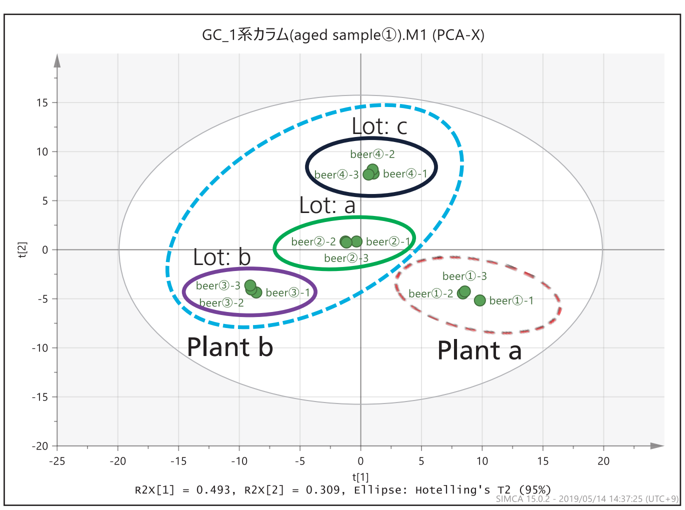


Figure 4 Score plot from GC-FID data

Table 6 Higher concentration compounds in each plant beer from loading plot

| Types of plant | Higher concentration compounds |
|---|---|
| Plant a | 3-Phenyllactic acid, Trehalose<br>Glyceric acid, Fructose 1-phosphate<br>Nonanoic acid, 2-Hydroxyisobutyric acid<br>Caproic acid, Glucose 6-phosphate<br>Sedoheptulose 7-phosphate<br>Mannose 6-phosphate<br>Glucose 6-phosphate |
| Plant b | Allose, Lysine, Tyramine, Methionine<br>Glutamic acid, Galactose<br>Phenylpyruvic acid, Tryptamine<br>2'-Deoxyuridine, Cystamine-d8, Uridine |

# Conclusions

- Score plot from GC-MS/MS and GC-FID successfully categorized five brands of beer, different plants and lots in same brand beer.
- From the loading plots in GC-MS/MS, we could identify important compounds which determine differences of beer brands, same brand beers brewed in different plants and product lots.
- This study suggest a new approach towards classification and visualization of beer quality.
- In the future, GC-FID potential for this filed will be tested in more detail.

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