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# A metabolomics approach to discriminate which compounds contribute to the sensory characters of coffee brews

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## Introduction

Coffee is among the most commonly consumed beverages in the world and numerous consumers find its pleasant flavors appealing. However, it remains unclear which compounds mainly contribute to the unique sensory characteristics of coffee. In this study, we used GC-MS metabolomics[1] to determine which compounds contribute to the sensory characteristics of coffee brews.

## Materials/Methods

A total of 28 samples, including five Arabica and two Robusta commodity coffees, were roasted to different extent. Each sample was then ground and brewed using a French press. The derivatization of the coffee brew and GC-MS analysis were conducted as reported previously[2]. The coffee brews were also evaluated for 12 sensory attributes. Each attribute was evaluated using a 10-point scale. The sensory evaluation and GC-MS datasets were subjected to multivariate analysis, principal component analysis (PCA), and partial least square regression (PLS-R).

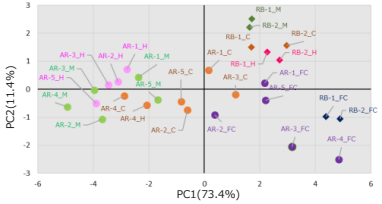


**Figure 1:** PCA score plot of sensory evaluation for 28 coffee samples((●) Arabica (◆) Robusta)

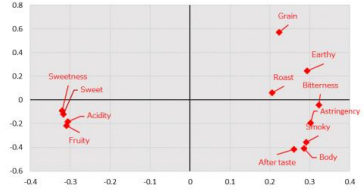


**Figure 2:** PCA Loading plot of 12 sensory attributes

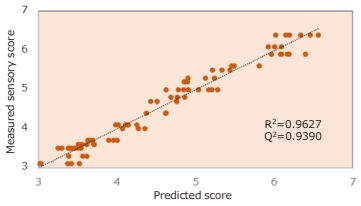


**Figure3:** PLS-R predicted model of acidity. Constructed from GC-MS compounds profile

**Table :** Key compounds contributing to the construction of acidity and sweet flavor predictive model (Top 3 in VIP Value)

| acidity | | sweet flavor | |
|---|---|---|---|
| Compound | VIP value | Compound | VIP value |
| Glyceric acid | 1.77 | D-Cellobiose | 1.83 |
| Galactose | 1.66 | Malic acid | 1.50 |
| Malic acid | 1.64 | Glyceric acid | 1.48 |

## Results/Discussion

The coffee sample-derived PCA score plot differentiated the groups based on the roasting degree and the coffee species (Arabica or Robusta) in the sensory evaluation results (Figs. 1 and 2).

The PLS-R model allowed us to predict the sensory scores of the coffee brews (Fig. 3).

Certain compounds were identified as contributors to each sensory attribute.
For example, Glyceric and Malic acids indicated a higher VIP value for the acidic taste and sweet flavor model (Table).

## Conclusion/Perspectives

We used GC-MS analysis and sensory evaluation to differentiate the compounds that contribute to the sensory attributes of coffee brews. In particular, we found that organic acids correlated with certain desired sensory attributes of the Arabica coffee brew (e.g., acidic taste and sweet flavor).

## References

[1] Pongsuwan et.al. J. Agric. Food Chem., 55, 231-236, 2007
[2] Jumhawan et.al. J. Agric. Food Chem., 61, 7994-8001, 2013