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Profiling of Metabolites Changes under Different Roasting Treatments of Arabica Coffee

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ABSTRACT

Roasting is part of post-harvest processing that impacts coffee's taste and odour. This study aimed at determining the changes in metabolites of Arabica coffee under three different roasting treatments i.e. light, medium and dark. The metabolites have been detected with Gas Chromatography-Mass Spectrometry. The obtained data were then statistically analyzed with multivariate analysis for a metabolomics approach. The cupping test (sensory analysis) was also used to compare the GC-MS analysis results. From the cupping test, it was concluded that the medium roasting treatments indicated the best score. The cupping test data were correlated with the multivariate analysis data referring to roasting conditions. Based on principle component analysis, the roasting process contributed various distributions of metabolites. A significant distribution of metabolites was discovered in medium roasting conditions, while less distribution occurred in dark conditions. The flavour compound as a group of esters might be responsible for significant components dominating medium roasted coffee. This study successfully elaborates the sensory analysis with analytical analysis to discover the suitable process for producing good quality coffee.

Key words: Metabolomics, sensory, quality, GC-MS, PCA

INTRODUCTION

Indonesia has many indigenous commodities of interest to be studied (Azima *et al.*, 2016, 2017, 2018). Coffee processing is one way that can be done to support coffee development (Saloko *et al.*, 2019). Coffee processing can also improve the quality and taste of coffee. Good coffee processing produces high-quality coffee beans. In general, there are two ways to process coffee cherries into coffee beans, namely, dry and wet processing. In addition, roasting is a process that plays an important role in the development of complex coffee flavours and aromas. In the roasting process involving heat, the heating principle uses atmospheric pressure and hot air as the medium. During the roasting process, physical changes and chemical reactions are very complex, so chemical components form the distinctive character of the coffee taste arises due to heat treatment (Fadri *et al.*, 2019). The roasting method consists of three levels: light roast, medium roast and dark roast (Agustini, 2020). The higher the roasting temperature, the blacker is the colour of the ground coffee produced, with more bitter the taste of the ground coffee, the higher the pH of the ground coffee, and the lower the water content. Muzaifa *et al.* (2020) reported that it was found that coffee during a light roast was light in colour, but during a medium roast and dark roast, it got darker. At the three stages of roasting, light, medium and dark roast, there is an increase in the shrinkage of the water content and the caffeine content. Based on the research by Pamungkas *et al.* (2021) the higher the roasting temperature, the lower the water content in Arabica coffee, the ash content in coffee decreased but was not significantly different, the fat content remained constant, the caffeine content increased and the coffee colour darkened. Seninde and Chambers (2020) stated that coffee roasted at a light roast level produced non-uniform coffee colour with a sour, grassy taste with an underdeveloped taste. The medium roast coffee provides a good balance of aroma and taste with a citrus

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flavour. Conversely, dark roast coffee produces coffee with a sensory profile with low acidity. The differences in many indicators reflected the quality of roasted coffee.

Although several studies have described differences in the quality of several roasting processes, only a few research has reported differences in roasting methods based on a metabolomics perspective. Metabolomics studies are relatively new studies that can concisely conclude but have outstanding accuracy. In metabolomics, the analysis could be conducted once, while the result will represent all metabolites due to the utilization of advanced analytical equipment such as gas chromatography-mass spectroscopy instrumentation. The conventional approach requires a very long time because each quality parameter must be analyzed with several different analytical methods. It was different with metabolomics in that analysis can be carried out comprehensively and statistically processed to obtain reliable conclusions (Syukri *et al.*, 2018, 2019, 2023; Thammawong *et al.*, 2019).

Therefore, in this study, the profiling of metabolites in Arabica coffee with three roasting conditions was mapped based on a metabolomics approach using gas chromatography-mass spectroscopy instrumentation. Moreover, the cupping test value was used as a reference, a coffee taste assessment technique acceptable to the public.

MATERIALS AND METHODS

Using a tub filled with running water, coffee cherries were cleaned and those that floated were separated. Out of 15 kg of coffee cherries, only dark red coffee cherries with 100% mucilage were selected. The outer skin of the coffee cherry was separated (pulping). After that, it was dried in the sun to get dry coffee beans with a moisture content of around 12%. The dried seeds were then collected after removing the husks.

The roaster (WExSuji, with a capacity of ±100 g) was used to preheat the beans for approximately 20 min. After that, 100 g of coffee beans were added to the roasting cylinder. The roasting treatment was as follows: low (light roast at temperature 185°C for 9 min), medium (medium roast at temperature 205°C for 11 min), and dark (dark roast at temperature 225°C for 15 min). The finished roasted coffee beans were removed from the roasting cylinder and cooled. The roasted coffee beans were ground in a grinder before being packaged.

Cupping is the process of observing the taste of coffee, finding out its personality, and tasting the coffee. Cupper is someone who does cupping. A trained person, also known as a Q grader, performs cupping. The cupping test uses a scale with four numerical values: good (6 - 6.9), very good (7-7.9), very good (8-8.9) and excellent (9 - 9.9). According to the cupping test, brewed coffee is classified as specialty coffee if the overall taste value is > 80 on a scale 100. The cupping test in this study was carried out by a Q grader with international certification.

An analytical technique was carried out to detect metabolites in coffee samples using GCMS. The metabolites detected with GCMS were derivatized with the compound N-Methyl-N-(trimethylsilyl)-trifluoroacetamide (MSTFA). In short, the metabolites present in the processed coffee were extracted by the Folch method and then derived. The derivatized compounds were then injected into the GCMS. GCMS conditions were set as standard conditions, among others, by using Helium gas as a carrier gas and a semi-polar column with a length of 30 m. The heating conditions of the column were adapted to a gradient from low temperature to high temperature (60 to 240°C). The MS detector was set to the default conditions on the device where the equipment was GCMS 2010 Ultra.

The samples were processed with multivariate analysis using Principal Component Analysis. The groups of the metabolites were distinguished according to the distribution of metabolites on each roasting condition.

RESULTS AND DISCUSSION

Fig. 1 indicates the distribution of detected metabolites in roasted coffee. In this study, the utilization of MSTFA as derivating agent successfully derived metabolites that had hidroxyl groups (Rini *et al.*, 2021). In other words, all metabolites including volatile and non-volatile hidroxyl groups were detected and analyzed during this measurement. The high number of metabolites were detected both on low and medium treatments, while only small number of metabolites showed on dark treatment. The high temperature on dark

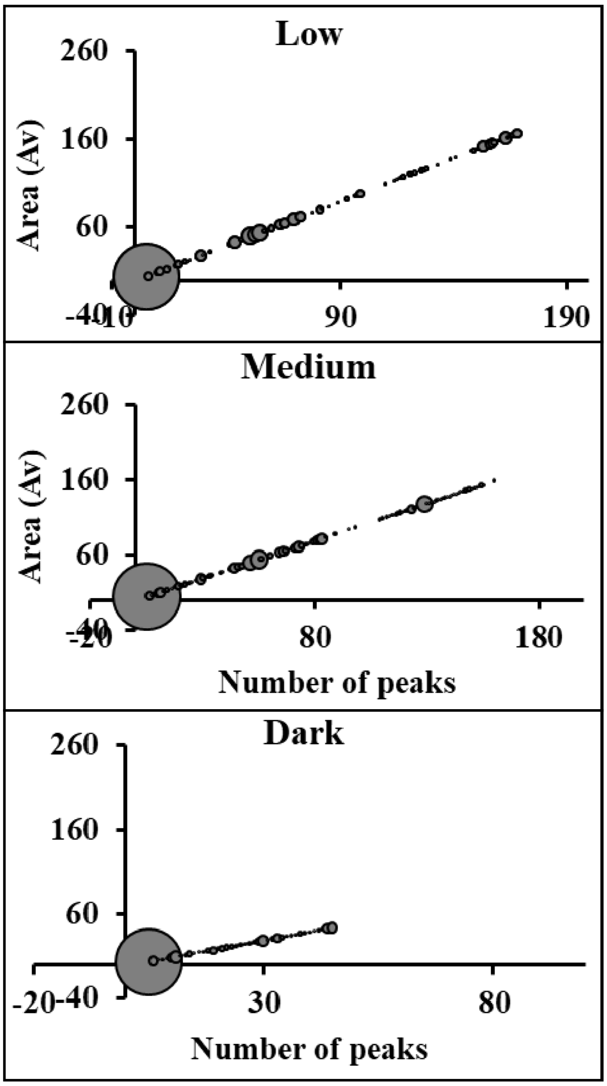

Fig. 1. Metabolites distribution in the roasted coffee as the result of GC-MS analysis.

treatment might cause the degradation of metabolites to the compound that had no hidroxyl groups that could derivate with MSFTA. The degradation might reduce the quality of roasted coffee. Moreover, according to this result, it can also be suggested that the compounds contained in the low and medium sample might induce the good flavour which affected good acceptability of low and medium roasted coffee (Münchow *et al.*, 2020). Fig. 1 had the limitation that the distribution of metabolites in low and medium treatment could not differentiate due to the similar trend; therefore, subsequent analysis was needed to be conducted.

Fig. 2 indicates the PCA results of treated samples according to the distribution of its metabolites. It can be informed that PCA had

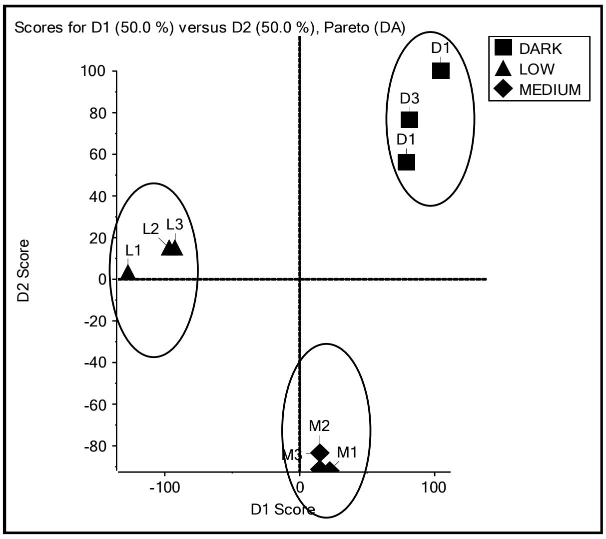

Fig. 2. PCA result of GCMS result of roasted coffee.

clearly separated the groups of treated sample. The distribution of metabolites on each treated sample was significantly diffrerent among three treated groups. It can be suggested that the metabolites on each treated sample were different and contributed to its taste and flavour. The roasting condition might induce different taste of produced coffee. The different tempareture during roasting condition clearly affected the existence of chemical compound in the coffee beans (Fikry *et al.*, 2019). The changes on chemical compound due to the roasting process might give positive or negative result where it can be corelated with the cupping test result.

Table 1 presents the cupping test result of three roasted coffee. The highest score of cupping test was obtained from the medium roasted coffee. It can be suggested that three different patterns of metabolites distribution of roasted coffee produced different quality of coffee. These data were related with the PCA result

Table 1. Score of cupping test of roasted coffee

Atrributes	Low	Medium	Dark
Uniformity	10.00	10.00	10.00
Clean cup	10.00	10.00	10.00
Sweetness	10.00	10.00	10.00
Aroma	7,25	7,75	7,51
Flavour	7,50	7,75	7,25
Aftertaste	7,50	8.00	7,50
Acidity	7,50	8.00	7,25
Body	7,75	7,75	7,50
Balance	7,25	8.00	7,50
Overall	7,50	7,75	7,25
Defects	0.00	0.00	0.00
Final score	82.00	85.00	81.50

that indicated the separation of roasted coffee due to the different distribution of its metabolites. Each coffee treatment received a final score of >80 in the cupping test done by professional panelists, according to the data. This demonstrated that every method of treating ground coffee produced specialty coffee (Tarigan and Randriani, 2023). The medium roast treatment in this trial produced the best final coffee score, which was 85. Suprising data were indicated by dark roasted coffee. Despite the compounds distributed in dark roasted coffee, the acceptability of dark roasted coffee was still in high score i.e. 81.5. These data might indicate that the number of chemical compounds did not affect the quality of roasted coffee. The type of chemical compounds might have dominant role in reflecting the quality of roasted coffee. The findings of the cupping test's description of the fragrance attribute revealed variations between each treatment. The aroma described by the aroma attribute became a burnt aroma as the roasting temperature and duration increased.

Fig. 3 displays the loading plot of PCA data produced by the statistical analysis of metabolites distribution in the roasted coffee. According to the basic PCA data shown on Fig. 2, in the region of medium roasted coffee, the presence of quininc acid and stearate compound might be resposible for the clusterization. Quinic acid seemed to be the main metabolite that played role to indicate the quality of roasted coffe in this study. As theoritically, quinic acid gradually rises after roasting as chlorogenic acid (CGA) undergoes a reduction change. The reason is that quinic acid is created when chlorogenic acid breaks down. Part of the quinic acid flavour will continue to degrade during roasting to produce a number of secondary chemicals, including phenol, catechol, hydroquinone, pyrogallol and certain diphenols, which are precursors for the coffee scent. Acidity is a crucial component of coffee flavors that shouldn't be overlooked (Seninde and Chambers, 2020). Depending on the type of coffee and how it is processed and roasted, there are dozens of organic acids found in coffee flavour. Moreover, in this study, another metabolite was also found which allegedly affected the quality or taste characteristics of medium roasted coffee. The propyl stearate compound was thought to be a flavour-forming component resulting from the medium roasting process. This information certainly needs further verification.

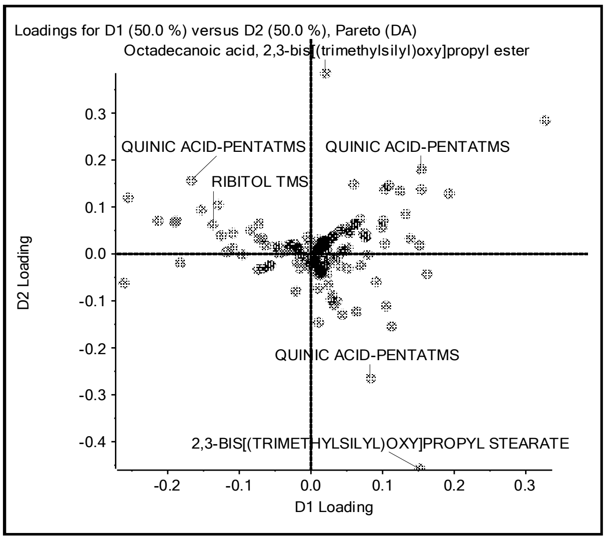

Fig. 3. PCA loading plots of metabolite distribution in roasted coffee.

CONCLUSION

Observation of the distribution of metabolites in roasted coffee with three treatments i.e. light roast, medium roast and dark roast was successfully carried out by a combination of analysis using GCMS instrumentation and statistical analysis. It is known that differences in roasting conditions have affected the distribution of metabolites in roasted coffee. Metabolites in coffee beans were easily affected by temperature conditions. In addition, it was also known that there was a relationship between metabolite distribution and taste testing which has shown that medium roasting conditions produced a specific taste and resulted in high acceptability of coffee. The findings from this study need to be studied further to confirm the compounds that are thought to be responsible for creating a good taste in medium roasted coffee products.

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