Available online at www.ijpcr.com
International Journal of Pharmaceutical and Clinical Research 2018; 10(3): 74-78

ISSN- 0975 1556

Research Article

The Cluster Analysis of Indonesian Coffee at Two Different Brewing Temperature Using FTIR-ATR (Fourier Transform Infrared – Attenuated Total Reflectance) Method Coupled with Chemometrics

Winingsih W*, Firmansyah A, Soebara Y S

Sekolah Tinggi Farmasi Indonesia (STFI) Bandung,Jl.Soekarno Hatta No. 354 (Parakan Resik) Bandung-Indonesia

Received: 18th Dec, 17; Revised 20th Feb, 18, Accepted: 8th Mar, 18; Available Online:25th Mar, 18

ABSTRACT

Coffees is an agricultural commodity that widely cultured at different region in Indonesia. From all Indonesian coffees, the best known coffee are from Aceh Gayo, Flores, Kintamani, Mandheling, Papua, Sidikalang, Toraja, Kerinci and Lampung. Those coffees have characteristic flavor that can only distinguish by the expert coffee taster. This study attempts to classify nine types of Indonesian coffee, therefore the different of those coffees tastes were studied from chemical aspect. For such purposes, the Fourier Transform Infra Red (FTIR) combined with chemometrics was used. In this case, FTIR was used to classify the coffees from various regions in Indonesia. The classification was conducted to the filtrate and residue of nine Indonesian coffees that was brewed at two different temperatures. The coffees samples studied were taken from nine regions in Indonesia, namely Aceh Gayo, Flores, Kintamani, Mandheling, Papua, Sidikalang, Toraja, Kerinci and Lampung. The chemometrics model used was principals component analysis (PCA) and cluster analysis (CA). From this study, the classification and similarities among the coffees that were brewed at two different temperatures can be known.

Keywords: Coffee, Spectrophotometer FTIR-ATR, Cluster analysis, Chemometrics.

INTRODUCTION

Natural product is varied depend on the localities and growing condition. Different geographical condition makes the variation chemical contain of Indonesian coffee that was studied. The former study result showed that they have different solubility, pH, and drying shrinkage value[1]. These value may also relate to the flavor of coffee.

Another factor that influences the coffee flavor is brewing temperature. Coffee grounds contain of volatile and non-volatile components, such as various oils, acids, and other aromatic molecules. Collectively, these compounds that are found in coffee grounds are referred to as "coffee solubles" and significantly contribute to coffee flavor. Brewing is the process of extracting these components from the grounds, so coffee beverages are technically a solution of coffee soluble and water. Temperature affects the solubility and volatility of the coffee soluble. Relative to brewing, solubility describes the ability of the soluble to dissolve out of the grounds and into the water; volatility refers to their ability to evaporate into the air[13]. With more coffee soluble extracted, hot brew coffees are described as more full-bodied and flavorful when compared to cold brew. Moreover, due to increased volatility with higher temperatures, the aromatics are more readily released from coffee, giving rise to that beloved scent of freshly-brewed coffee. This research attempt to analyze the cluster of the filtrate and the residue of coffee from nine regions in Indonesia that brewed at 80ºC and 25ºC. The cluster of the coffee can describe the similarities between the studied coffee base on their physical chemical properties which is related to their flavor.

The methods that usually used for such purposes are chromatography techniques such as High Performance Liquid Chromatography (HPLC), Gas Chromatography (GC), or Gas Chromatography-Mass Spectrophotometry (GC-MS) and Thin Layer Chromatography (TLC)[2].

Unfortunately, these methods are impractical and laborious. In addition, the method employing many reagents is not environmentally friendly[2]. Based on this, more practical methods of analysis are required. Because of those reasons, Fourier transformed infrared spectrophotometry (FTIR) is the preferred method used. It offered some benefits of its usage, namely simple operation, faster time analysis and environmentally friendly because of its little usage of reagents[3,5].

The FTIR spectrum resulted is complicated and hard to interpret. Thus, to assist data interpretation, chemometrics model is applied. The chemometrics model used was Principal Component Analysis (PCA) and Cluster Analysis (CA)[3].

PCA and CA, an unsupervised pattern recognition, was used to find out the main source of variability present in the data sets. It was used to detect cluster formatting and to establish relationship between object and variable. Among others, PCA is the most often used method of handling multivariate data prior knowledge about the studied samples**.** Thus, the application of chemometrics techniques will greatly improve the quality of spectrum obtained[6].

**Author for Correspondence: Winingsih341@gmail.com*

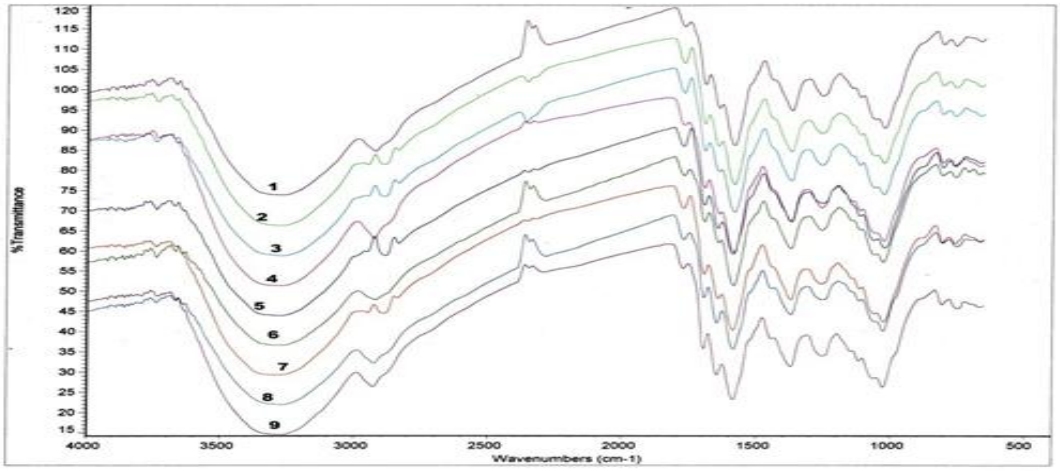


Figure 1: FTIR spectrum of coffee residue at 25ºC ; 1. Aceh gayo; 2. Flores; 3. Kintamani; 4.Mandailing; 5.Papua ; 6.Sidikalang; 7.Toraja ; 8. Kerinci; 9. Lampung.

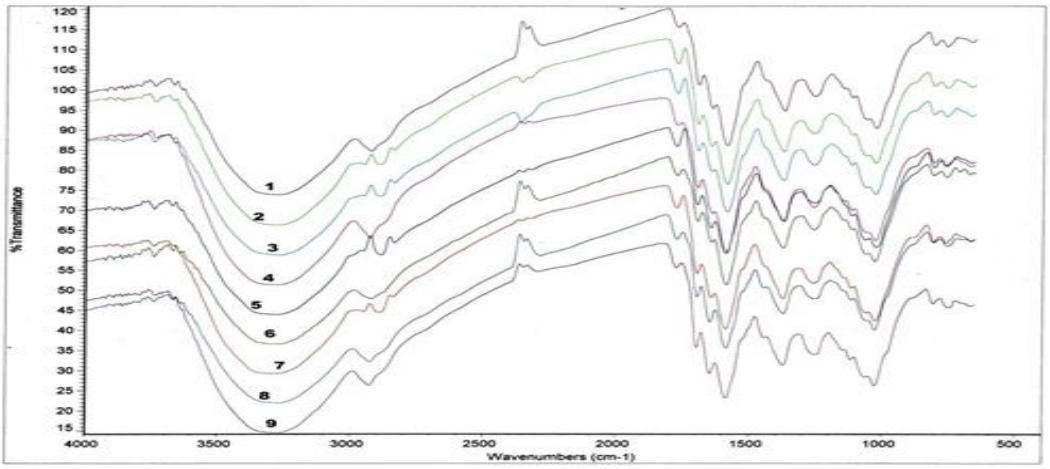


Figure 2: FTIR spectrum of coffee residue at 80ºC ; 1. Aceh gayo ; 2. Flores ; 3. Kintamani; 4.Mandailing; 5.Papua ; 6.Sidikalang; 7.Toraja ; 8. Kerinci; 9. Lampung.

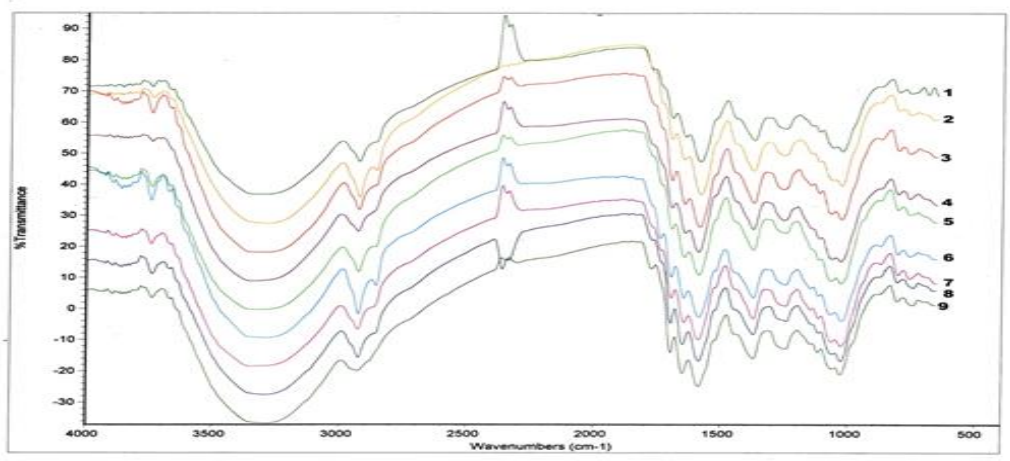


Figure 3: FTIR spectrum of coffee filtrate at 25ºC ; 1. Aceh gayo; 2. Flores; 3. Kintamani; 4.Mandailing; 5.Papua ; 6.Sidikalang; 7.Toraja ;8.Kerinci; 9. Lampung.

MATERIALS AND METHOD

Equipment

Equipment used in this study was FTIR Spectrophotometer (Thermo Scientific Nicolet iS5) equipped with ATR (attenuated total reflectance) and ZnSe crystal

Material

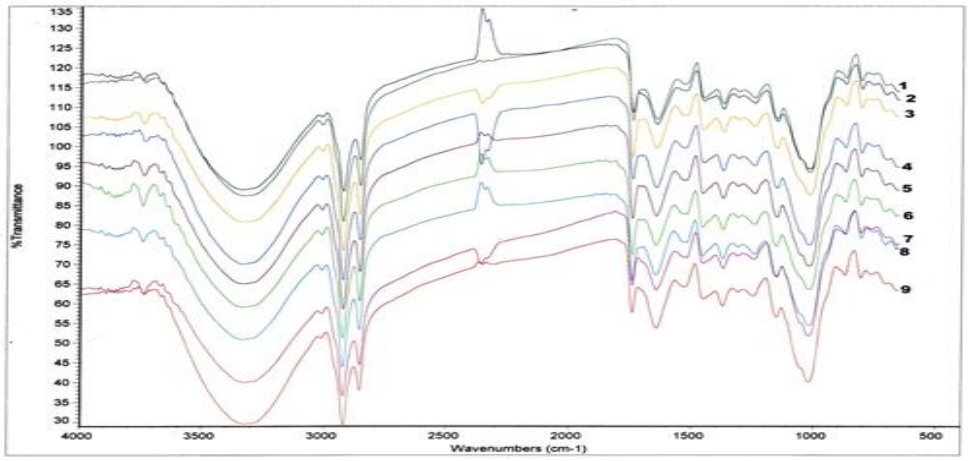
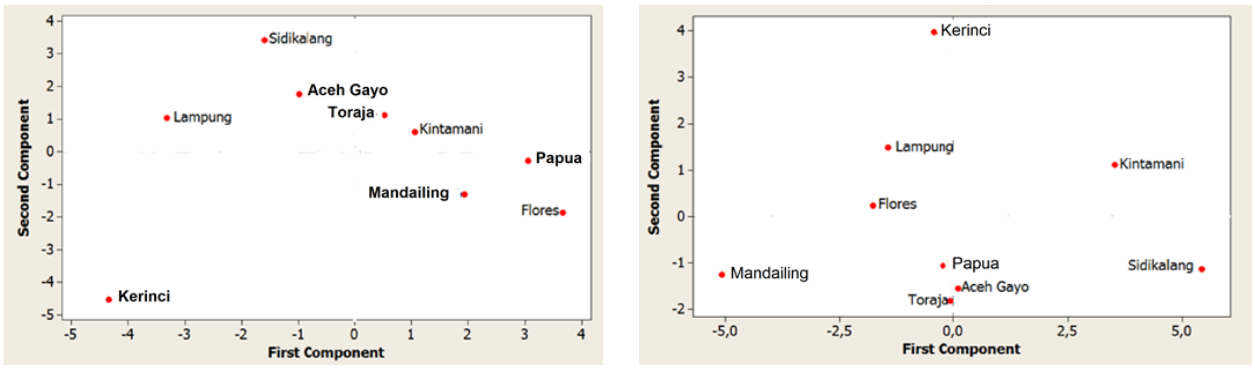
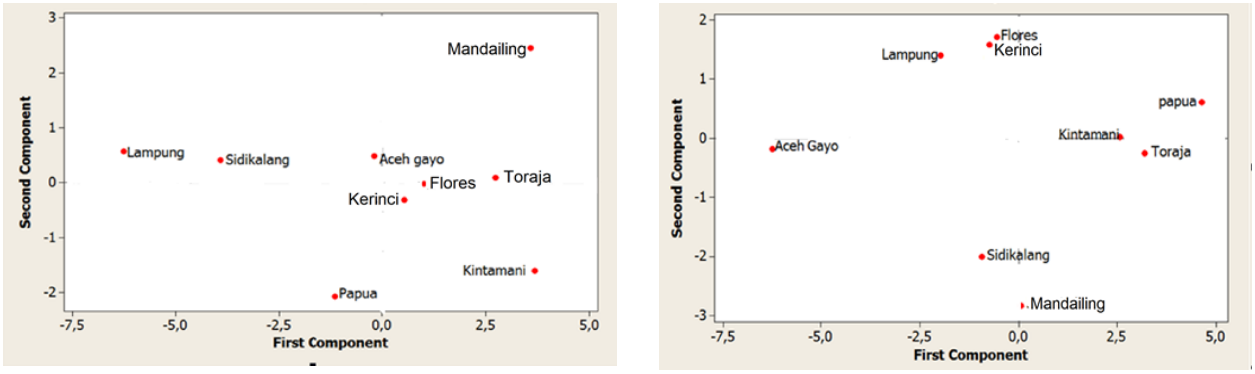


Figure 4: FTIR spectrum of coffee filtrate at 80ºC ; 1. Aceh gayo ; 2. Flores ; 3. Kintamani; 4.Mandailing; 5.Papua ; 6.Sidikalang; 7.Toraja ; 8. Kerinci; 9. Lampung.



A B

Figure 5: The result of PCA analysis of coffee residue. A: at 25ºC B: at 80º



A B

Figure 6: The result of PCA analysis coffee filtrate. A: at 25ºC; B: at 80ºC.

Materials used are coffee powder from nines region of Indonesia was purchased from Terminal kopi. The only reagent that was used in this study was distilled water

Sample Preparation

The samples were brewed with distilled water at 25ºC and 80ºC, in which the residues were dried in an oven at a temperature of 40^{0}C, and the filtrates were evaporated until dried and became powder.

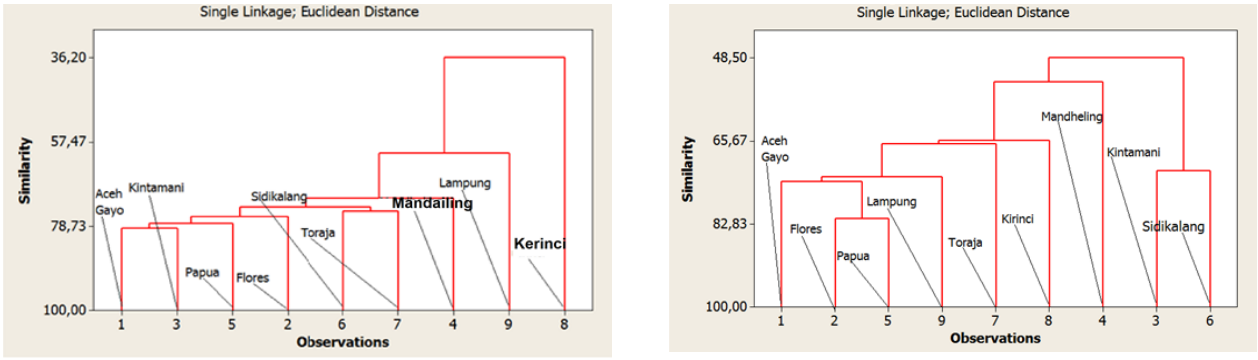
Determination of the main FTIR spectrum of the test sample and chemometrics study

Spectrum determination conducted to filtrate and residue of coffee brewed at 25ºC and 80ºC. Then, the manipulation of the spectrum was conducted by smoothing 9 (17.356 cm^{-1}) to each of the resulted spectra.

The absorbance of 15 wavenumbers (3800-800 cm^{-1}) was analyzed by chemometrics model using minitab software. The chemometrics model used was Principal component analysis (PCA) and cluster analysis (CA).

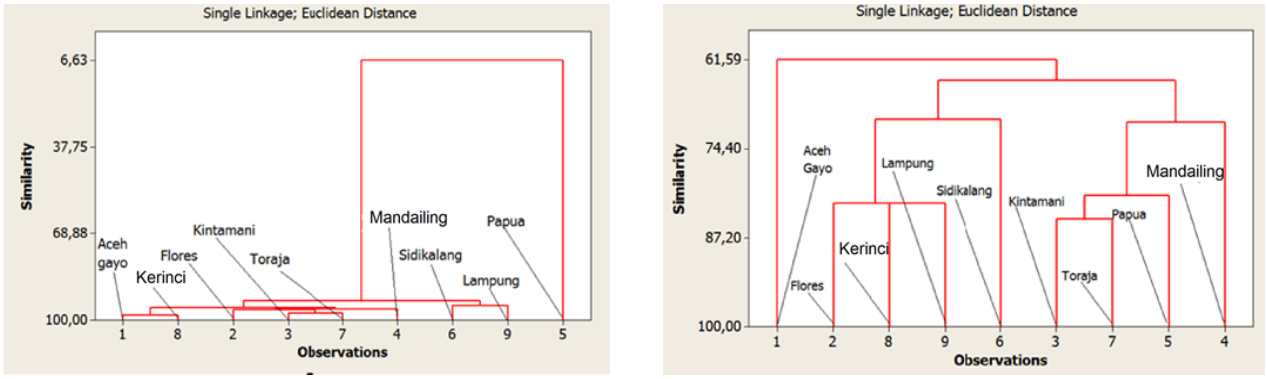
RESULT AND DISCUSSION

The result of spectrum determination of the residue and filtrate of coffee brewed at temperature of 25ºC and 80ºC was shown at figure 1-4. From that pictures, it can be seen that they have similar peaks with different intensity



A B

Figure 7: The result of CA analysis of coffee residue. A: at 25ºC; B: at 80ºC



A B

Figure 8: The result of CA analysis of coffee filtrate. A: at 25ºC ; B: at 80ºC

indicating the difference of coffee soluble contain. The influence of brewing temperature can be seen from the spectrum in figure 3 and 4 that showed more intense peak at wavelength 3000-2500. The cluster and similarity identification of the coffees cannot be find out by using the FTIR spectrum only, hence, there should be further analysis of the spectrum results using chermometric method such as principal component analysis (PCA) and cluster analysis (CA).

Principal component analysis (PCA) and cluster analysis (CA) was conducted by collecting all the data absorbance at several wavenumbers of each coffee. The result of PCA coffee residue shown in figure 5, the result of PCA coffee filtrate is shown in figure 6. The outcome of principal component analysis (PCA) is a score plot which is the distance between the points of score plots shows the closeness between each coffee whereas CA produced a dendogram that can show the similarity percentage of each coffee. The greater the similarity percentage, the greater similarities owned by the coffee. The result of cluster analysis is shown in figure 7 and 8.

Base of those two chemometrics studied it is known that the difference in brewing temperature produce different coffee cluster. For example, Aceh Gayo coffee residue which is brewed at 25ºC has closed similarity with Toraja coffee, but if it was brewed at 80ºC it has closeness with Toraja and Papua coffee (figure 5 and 7). The same result also occurred for the filtrate (figure 6 and 8), at 25ºC the Aceh Gayo coffee has closeness to Flores, Kerinci and Toraja coffee but when it was brewed at 80ºC, Aceh Gayo coffee has no closeness with any coffee. This mean that when Aceh Gayo coffee was brewed at 25ºC the taste assume will be similar with Toraja, Kerinci and Flores coffee, but if it was brewed at 80ºC the taste of those coffees was very different.

From this study it was found that FTIR – chemometrics technique has succeed to cluster of Indonesian coffee from nine region that brewed at two different temperature base on their physicochemical properties. Since the physicochemical properties related to their flavor, this simple method can be used to predict the similarity of coffee taste without involving a coffee taster.

ACKNOWLEDGEMENT

The author is very grateful to Sekolah Tinggi Farmasi Indonesia Bandung for the facilities that have been provided during this research.

REFERENCES

1. Firmansyah,A.,Winingsih,W.,Soebara,YS., The Utilization of FTIR (Fourier Transform Infrared) Combined with Chemometrics for Authentication of Indonesian Coffee Powder, *International Journal of Pharmaceutical and Clinical Research*,2017;9:210-13.
2. Sim, C. O.et.al, Assesment of Herbal Medicines by Chemometric-Assisted Interprestation of FTIR Spectra, *Journal Of Analytica Chimica ACTA*,2004.

3. Rohman, A.,Arsanti,L.,Erwanto Y., Pranoto,Y., The Used of Vibrational Spectroscopy and Chemometrics in The Analysis of Pig Derivatives for Halal Authentication, *International Food Research Journal*,2016;23: 1839-48.
4. A.F. Nurrulhidayah,Y.B. Che Man,H.A. Kahtani,and A. Rohman, Application of FTIR Spectroscopy Coupled with Chemometrics for Authentication of Nigella Sativa Seed oil,*Spectroscopy*, 2011;25 :243-50.
5. Doughlas F.B.,Ana Lucia D.S.M.F.,Da-Wen Sun.,Suzana L.N., Elisa Y. H., Application of Infrared Spectral Techniques on Quality and Compositional Attributes of Coffee : An Overview, *Food Research International*, 2014;61:23-32.
6. A.Bansal,Vikas C., Ravindra K.R.,Simant S., Chemometric : A New Scenario in Herbal Drug Standardization, *Journal of Pharmaceutical Analysis*, 2014;4:223-33.
7. Almeida, P., Cherubino, A.P.F., Alves, R.J., Dufossé, L. & Gloria., M.B.A., Separation and Determination of The Physico-chemical characteristics of Curcumin, Demethoxycurcumin and Bisdementhoxycurcumin, *Food Res Int*, 2005;38: 1039-1044.
8. Zhang, J.S., Guan, J., Yang, F.Q., Liu, H.G., Cheng, X.J. & Li, S.P., Qualitative and Quantitative Analysis of Four Species of Curcuma rhizomes Using Twice Developement Thin Layer Chromatography, *JPharmaceut Biomed*, 2008; 48; 1024-1028.
9. Anderson, A.M., Mitchell, M.S. & Mohan, R.S., Isolation of Curcumin fromT Tumeric, J Chem Educ,2000; 77: 359-60.
10. Cahyono, B., Muhammad, D. & Limantara, L., Pengaruh Proses Pengeringan Rimpang Temulawak *(Curcuma xanthorrhiza* ROXB) Terhadap Kandungan dan Komposisi Kurkuminoid, *Reaktor*, 2011;13: 165-171.
11. Jiang, A., Somogyi, A., Jacobsen, N.E., Timmermann, B.N. & Gang, D.R.,Analysis of Curcuminoids by Positive and Negative Electrospray Ionization and Tandem Mass Spectrometry Rapid Commun Mass SP,2006;20: 1001-1012.
12. Lee, J.H. & Choung, M.G., "Determination of Curcuminoid Colouring Principles in Commercial Foods by HPLC", *Food Chem*, 2011;124: 1217- 22.
13. Jumhawan, U.; Putri, S. P.; Yusianto, Marwana, E; Bamba, T.; and Fukusaki, E., Selection of Discriminant Markers for Authentication of Asia Palm Civet Coffe (Kopi Luwak): A Metabolomics Approach, *J. Agric. Food Chem*., 2013;61: 7994-800.