Pharmaceutical and Biomedical Sciences Journal
Volume 2(2), 2020, 49-52

Chemical Compounds of Coffee Ground and Spent Coffee Ground for Pharmaceutical Products

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Received: 24 November 2020; Accepted 25 February 2021

Abstract: Coffee is one of the most valuable primary products in world trade. Coffee production generates a lot of coffee waste such as spent coffee grounds. The chemical components of the coffee ground and spent coffee ground were caffeine and chlorogenic acid. These components were important to apply in pharmaceuticals. This research conducted the identification of functional groups of coffee grounds and spent coffee grounds and analysis of the active compounds of caffeine and chlorogenic acid in the sample. Both samples have the same infrared spectrum and contain the main functional groups O-H, C-N, and C-H. The active substances in the spent coffee grounds were found to be caffeine 0.35% and chlorogenic acid 0.16%, while in coffee ground coffee before brewing it was obtained 1.41% caffeine and 1.50% chlorogenic acid. The waste of spent coffee grounds has a potential component and it can be used in pharmaceuticals.

Keywords: Caffeine, chlorogenic acid, spent coffee ground

1. INTRODUCTION

Coffee is one of the most important agricultural commodities and the most consumed beverage in the world. Coffee contains more than 1500 chemicals, 850 volatiles, and 700 dissolved compounds. When coffee is extracted in water, most of the hydrophobic compounds including lipids, triglycerides, and fatty acids remain. The structure of lignin, phenolics, aroma-producing essential oils are also present in coffee (Blinova, *et al.*, 2017). Coffee waste, which is usually called spent coffee ground (SCG), is waste that comes from brewing coffee. There are ± 0.91 g of coffee grounds produced per 1 g of ground coffee and ± 2 kg of used coffee grounds are produced for every kilogram of instant coffee made (Blinova, *et al.*, 2017). The manufacture of espresso coffee drinks produces 45% of the waste produced and disposed of as solid waste (Stylianou, *et al.,* 2017).Spent coffee ground contains 12.4% cellulose, 39.1% hemicellulose, 3.6% arabinose, 19.07% mannose, 16, 43% galactose, 23.9% lignin, 2.29% fat, 17.44% protein and 60.49% of total dietary fiber (Cruz, *et al.*, 2014). This composition is very interesting and needs to be separated from the waste of the spent coffee ground. The potential contained in the spent coffee ground is beverage products (Mussatto, *et al.*, 2001) and antioxidants (Panusa, *et al.*, 2013).

The biological activities of coffee have been mainly attributed to terpenes, alkaloids, and phenolic compounds. The main alkaloid is caffeine (1,3,7 trimetylxantine) (Stefanello, 2019). Caffeine, 1,3,7-trimetyl-xantine, a pure alkaloid, is the most popular component recognized in coffee and coffee products. Although the caffeine content in coffee waste is lower than in coffee beans, a large amount of caffeine remains. The caffeine content for arabica ranges from 0,9 and 1,6 %, robusta (1,4-2,9 % (Vega, *et al.*, 2015). Chlorogenic acids (CGA) are abundant phenolic compounds in coffee. Despite the potential bio-pharmacological properties attributed to these compounds, little knowledge about their bioavailability in humans. CGA is formed by the esterification of hydroxycinnamic acid (Monteiro, 2017). CGA an important biological active dietary polyphenol is produced by certain plant species and a major component of coffee. The biological properties of CGA in addition to its antioxidant and anti-inflammatory effect. The health benefits of CGA including antidiabetic, anti-carcinogenic, anti-inflammatory (Tajik, *et al.*, 2017; Macheiner, *et al.*, 2019). The analysis of chemical compounds in coffee grounds and spent coffee grounds is important to be investigated because it can inform the potential use in pharmaceuticals. This information can be used to utilize the waste of coffee products in pharmaceuticals. This study aims to analyze chemical compounds in the coffee ground and spent coffee ground. The analysis consists of a functional group with infrared spectroscopy, caffeine, and chlorogenic acid with high-performance liquid chromatography.

2. MATERIAL AND METHODS

2.1. Identification of functional groups

Characterization of coffee ground and spent coffee ground were achieved by infrared analysis. FTIR analysis was used for the identification of the functional group of samples including organic compounds. The transmission infrared spectra were recorded in the 4000 cm^{-1} to 700 cm^{-1} range using ALPHA BRUKER-IR.

2.2. Analysis of caffeine and chlorogenic acid

Analysis of caffeine and chlorogenic acid (5-CQA and 3-CQA) was performed using HPLC. A 10 mg / mL coffee extract solution was analyzed using a reverse-phase HPLC column. The mobile phase consisted of solvent A (50 mM acetic acid in distilled water and solvent B (50mM acetic acid in acetonitrile) using the following gradient elution method: 0–30.0 min, 0–20% (v / v) of B; 30.0– 45.0 min, 20–35% (v / v) of B; 45.0–50.0 min, 35–80% (v / v) of B; 50.0–50.1 min, 80–5% (v / v) of B; and 50.1–60 min, 0% (v / v) of B. The injection volume of the coffee husk extract sample was 10 µL and the flow rate was 1.0 mL / min. Caffeine and chlorogenic acid were detected at absorption wavelengths of 270 and 325 nm, respectively. Caffeine and chlorogenic acid were identified by comparing the retention time and chromatogram of standard solutions (Diao *et al.*, 2010).

3. RESULTS AND DISCUSSION

Analysis of the components of ground coffee and spent coffee ground waste was carried out using infrared spectroscopy and high-performance liquid chromatography.

3.1. Identification of functional groups

Preliminary tests on ground coffee and spent coffee grounds were analyzed using infrared spectroscopy to see the composition of compounds contained in coffee ground and spent coffee ground by identifying the functional groups in the sample. In the spent coffee ground, the intensity is high at the wave number 3346 cm^{-1} which is the O-H group. The intensity obtained is higher than coffee grounds. This is because the polarity nature of the spent coffee ground is increasing due to the interaction with water during brewing so that it forms bigger hydrogen bonds. In both coffee samples, the C-N peaks were quite high in intensity. The C-N group is a functional group found in caffeine compounds so that from the identification of the functional groups, it can be seen that the samples have a functional group for caffeine compounds. The results of FTIR analysis can be seen in Figure 1and information on functional groups contained in both samples can be seen in Table 1.

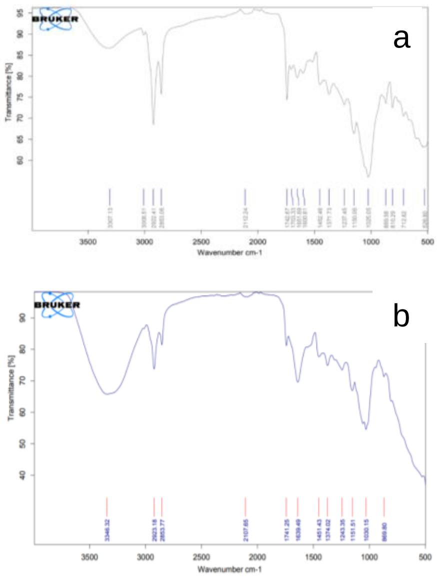

Figure 1. The Infrared spectrum of coffee ground (a) and spent coffee ground (b)

Table 1 . Identification of functional groups

Coffee ground		*Spent coffee ground*	
Wave number (cm $^{-1}$)	Functional groups	Wave number (cm $^{-1}$)	Function al groups
3307	O-H	3346	O-H
2922	C-H	2923	C-H
2853	C-H	2853	C-H
1742	COOR	1639	COOR
1025	C-N	1030	C-N

Based on the research, it can be seen that the spectrum patterns found in coffee grounds and spent coffee grounds are the same. This shows that the components of the compounds contained in the coffee ground before and after brewing are still principally the same. The chemical composition contained in the coffee ground still contains active substances contained in coffee. The main peaks are obtained at the wavenumbers 3307 cm^{-1} and 3346 cm^{-1} which are the peaks for the hydroxyl groups. The shape of the peak widens due to the hydrogen bonding of the compound. This hydroxyl group is a functional group which is a group of polyphenol or antioxidant compounds found in ground coffee and coffee grounds. The peak in the wavenumber 2915-2935 cm^{-1} is an identification for the asymmetric methyl C-H functional group (Coates, 2006). This functional group is an extension of the carbon chain which is the organic compounds present in the sample. The wavenumbers that appear in the range 2865-2845 cm^{-1} are asymmetric methyl groups. This class of compounds is usually found in caffeine compounds in coffee. Wavenumber with a range of 1750-1725 cm^{-1} is a group of ester compounds identified in the structure of chlorogenic acid compounds. The results of the identification of coffee grounds functional groups showed that the active substances found in coffee grounds were still the same as those in the original coffee and did not experience structural changes or degradation during brewing.

3.2. Analysis of caffeine and chlorogenic acid

Further identification of the main active substance in coffee, namely caffeine. The levels of caffeine compound in the coffee ground and spent coffee ground can be seen in Figure 2.

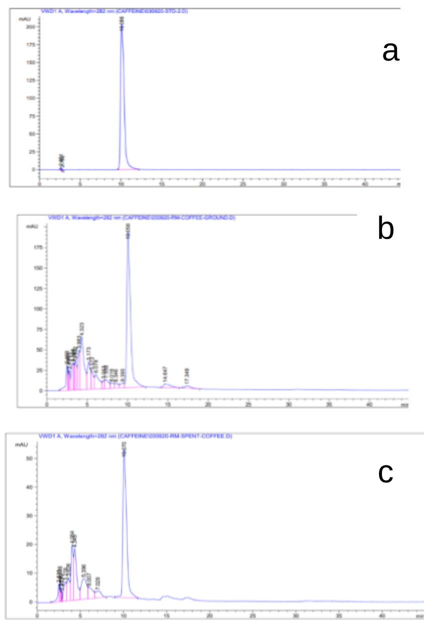

Figure 2. Chromatogram of caffeine analysis a) caffeine standard; b) coffee ground; c) spend coffee ground

Based on Figure 2, it can be seen that the spectrum from the high-performance liquid chromatography

(HPLC) analysis of the coffee ground and spent coffee ground shows the identification of caffeine compounds in the sample. The chromatogram results showed that the spent coffee ground still contained caffeine compounds as well as the coffee ground. Standard caffeine has a retention time of 10.086 minutes. Coffee grounds and spent coffee grounds have retention times of 10.056 and 10.070 minutes, respectively. The caffeine content obtained can be seen in Table 2.

Table. 2. Caffeine and chlorogenic acid content in coffee ground dan spent coffee ground

Sample	Caffeine (%)	Chorogenic acid %
Coffee ground	1,41	1,50
Spend coffee ground	0,35	0,16

Based on Table 2, it was found that the caffeine content in the coffee powder was 1.41% and in the coffee grounds was 0.35%. Based on these data, it can be seen that in the coffee brewing process, not all caffeine is extracted. The waste coffee grounds each left almost half of the caffeine content. The coffee grounds of the spent coffee ground still contain the active substances needed.

4. CONCLUSION

Based on the research that has been done, it can be concluded that the results of the initial identification of spent coffee ground are compared to spent coffee ground. The samples have active substances like caffeine and chlorogenic acid The waste of spent coffee ground has potential components and it can be used in pharmaceuticals.

5. ACKNOWLEDGMENT

We thank the Pusdiklat Ministry of Industry, Republic of Indonesia for the financial support of this research (SK No.226/BPSDMI.3/VIII/2020.

6. REFERENCES

Blinova, L., Sirotiale, M., Bartosova, A. and Soldan, M. (2017) ‘Utilization of waste from coffee production’, Research Papers, Faculty of Material Science and Technology in Trnava, Slovak University of Technology, Bratislava, 2017, 25 (40), 91-101.

Coates, J., (2006) ‘Interpretation of infrared spectra, a practical approach, encyclopedia of analytical chemistry’, Willey & sons Ltd, 1-23.

Cruz, R. (2014) ‘Coffee by-product: Sustainable Agro-Industrial recovery and Impact on Vegetables Quality’, Dissertation, Universidade de porto.

Diao, F., Dong, F., Wang, Q., Liu, W., Guo, D., Cui, X. (2010) ’Thianine, EGCG, and Caffeine determined by HPLC, National Center for Biotechnology Information, 39(1), 107-109.

Macheiner, l., Schemidr, A., Schreiner, M. and Mayer H,K. (2019) ‘Green coffee infusion a source of caffeine and chlorogenic acid’, Journal of Food Composition and Analysis, 84, 1-8.

Mussatto, S.I., Machado, E.M.S., Carneiro, L.M. and Teixeira, J.A. (2012) ‘Sugars metabolism and ethanol production by different yeast strains from coffee industry waste hydrolysates’, Applied Energy, 92,763-768.

Monteiro. M., Farah, A., Perrone, Truge, L.C. and Donangelo, C. (2007) ‘Chlorogenic acid compounds from coffee are differentially absorbed and metabolized in humans’, The Journal of Nutrition, 137 (10), 2196-2201.

Panusa, A., Zuoro, A., Lavecchia, R., Marrosa, G. and Petrucci, R. (2013) ‘Recovery of natural antioxidant from spent coffee ground’, Journal of Agricultural and Food Chemistry, 61, 4162-4168.

Stylianou, M.A., Agapiou, A., Omirov, M., Vyrides, I., Loannides, I. M., Maratheffis, G. and Fasoula, D.A. (2017) ‘Potential environmental application of spent coffee ground’, Proceeding of the 5th International Conference on Sustainable Solid Waste Management.

Stefanello, N., Spanevello, R.M., Passamonti, S., Porciuncula, L., Bonan, C.D., Olabiyi, A.A., Rocha, J.B.T., Assmann, C.T., Morch, V.M. and Schetinger, M.R.C. (2019) ‘Coffee, caffeine, chlorogenic acid, and the purinergic system, Food and Chemical Toxicology, 12, 298-313.

Tajik, N., Tajik, M., Mack, I., Enck, P. (2017) ‘The potential effects of chlorogenic acid, the main phenolic component in coffee on health a comprehensive review of the litelature’, European Journal of Nutritions, 56, 2215-2244.

Vega, R..C., Piria, G.C, Castaneda, H.A.V, Oomah, B.D. (2015) ‘Spent coffee grounds: A review on current research and future prospects’, Tends in Food & Technology, 45, 24-36.