*Available online www.jocpr.com*

**Journal of Chemical and Pharmaceutical Research, 2016, 8(3):348-352**

**Research Article**

**ISSN : 0975-7384**
**CODEN(USA) : JCPRC5**

# Application of principal component analysis (PCA) in discriminant process on ethanol extract of Majapahit, Pegagan, Mangosteen Rind and its scavenging activity of free radicals DPPH

**Mustofa Ahda**

*Department of Pharmacy, Ahmad Dahlan University, Yogyakarta, Indonesia*

---

**ABSTRACT**

*Principal Component Analysis (PCA) is a method to discriminant process a some active compound in herbal plants. The aims of this study were to compare the quality of ethanol extract of majapahit (Cresintia cujete), pegagan (Centella asiatica), and mangosteen rind (Garcinia mangostana) and also will determinant the discriminant between the herbal plants. Basic discriminant process were all component from active compound in the ethanol extract of the herbal plants. The results show that the discriminant process of ethanol extract from mangosteen rind, pegagan, and majapahit using Principal Component Analysis (PCA) can be distinguished. This discriminant result as an evidence for the active compound in the extract has different. This distinction is supported by the antioxidant activities of extract ethanol of mangosteen rind has antioxidant activity better than ethanol extract of pegagan and majapahit. The scavenging ability of DPPH from ethanol extract of mangosteen rind, pegagan and majapahit were 40.1 ug/mL, 172.1 ug/mL and 153 ug/mL respectively.*

**Keywords**: Discriminant Process, PCA Analysis, Antioxidant Ability

---

## INTRODUCTION

The development of herbal medicine is an interesting topic. Many researchers were developing and finding from plants which it have efficacy for disease treatment. Some plants have been found and have ability in pharmacology activity. In general, the testing process for quality the herbal plants which include two parameters. These are specific and non-specific parameters. The specific parameters include profile thin layer chromatography (TLC) the active compound and the secondary metabolites levels. The non-specific parameters include the residual water levels, ash content, ash soluble acid, microbiological parameters and heavy metals levels such as Pb , Cd , As, Hg [1].

The specific parameters such as identification of the flavonoids on mangosteen [2], the identification of the derivatives xanton and anthraquinone on mangosteen [3], or identification the flavonoid and santorizol on ginger plants [4]. Besides that, the quality of herb medicine can be seen from materials toxicity. According to [5] mentions that the materials toxicity include pesticide residues, heavy metals, patogen microbial contaminant. Therefore, many research determinant the heavy metals content in herbal samples. [6] have determined the heavy metals content in samples of herbal medicine. The same study by [7] who conducted the analysis of heavy metals content in traditional chinese herbal medicine by using a microwave plasma-atomic emission spectrometry (MP-AES). The effectivity and efficacy of the herbal plants are usually influenced the active compound and materials toxicity.

The development and using of herbal plants for medicine has more problems such as the consistency of active compound and materials toxicity. The consistency of active compound in herbal have variation in the interspesies or intraspesies, environmental factors, harvesting time and post harvesting factor [8]. The methods used for detection of active compounds in material herbal by analyzing the chemical compounds. Therefore, it was developed for analysis the active compound which can be used for authentication in herbal plants.

The aims of this study were to distinguish the herb extract from pegagan, majapahit and mangosteen rind using FTIR spectrometry combined Principle Component Analysis (PCA). The use FTIR spectrometry in discriminant process, because it has capability to phytochemical studies in fingerprinting field. Near infrared spectroscopy (NIRS) can be used in a qualitative and quantitative analysis on the product TCM (Traditional Chinese Medicinal) [9]. [10] reported that the FTIR spectroscopy with chemometrics can be used for quality control the herbal samples with fast authentication. The chemometrics can evaluate the herb quality and be used to optimize the experimental procedure, useful for information the extract and pre-treatment of fingerprints [11]. Therefore, this study also compared the antioxidant activity for scavenging activity of free radicals DPPH.

## EXPERIMENTAL SECTION

### Materials

The raw material are used mangosteen Rind (Yogyakarta fruit market), Pegagan, and Majapahit (herbs market of Merapi pharma), ethanol absolute, methanol, distilled water, DPPH solution 1 mM.

### Sample Preparation

The mangosteen rind dried in open air for 7 days. The pegagan and majapahit dried in an oven to 50 °C for 7 days. All ethanol extracts from all herbal plants used in powder form.

### Extraction Process of Medicinal Plants

One hundred grams powder of herbs macerated with absolute ethanol 400 ml for 24 hours with stirring. After maceration for 24 hours, the solution is filtered by a vacuum to separate the pulp and filtrate. Then the solvent evaporated with a rotary vacuum evaporator and dried to obtain a dry extract. The herbal plants used are pegagan, majapahit and mangosteen rind.

### Determination the Scavenging Activity of Free Radicals DPPH

Antoxidant activity of DPPH adopted from [12]: Determination of scavenging activities of free radical of DPPH carried out by taking 1.0 ml of ethanol extracts of herbal plants and 1.0 mL of DPPH solution 1 mM and mixing homogenously. so, its measured at a wavelength of 517 nm using a spectrophotometer Uv-vis after 30 min.

### Data Processing with Principle Component Analysis (PCA)

The Data processing of FTIR spectrum with Principle Component Analysis (PCA) analysis using software The Unscrambler 10 (Camo software).

## RESULTS AND DISCUSSION

### The FTIR Spectrum Characterization of Ethanol Extract from Pegagan, Majapahit and Mangosteen Rind

The extract ethanol from different herbal have a different composition in the active compounds. The differences composition of active compounds may altered the effectivity, its used as a herbal medicine. The different of active compounds were characterized using FTIR spectrometry (Figure 1).

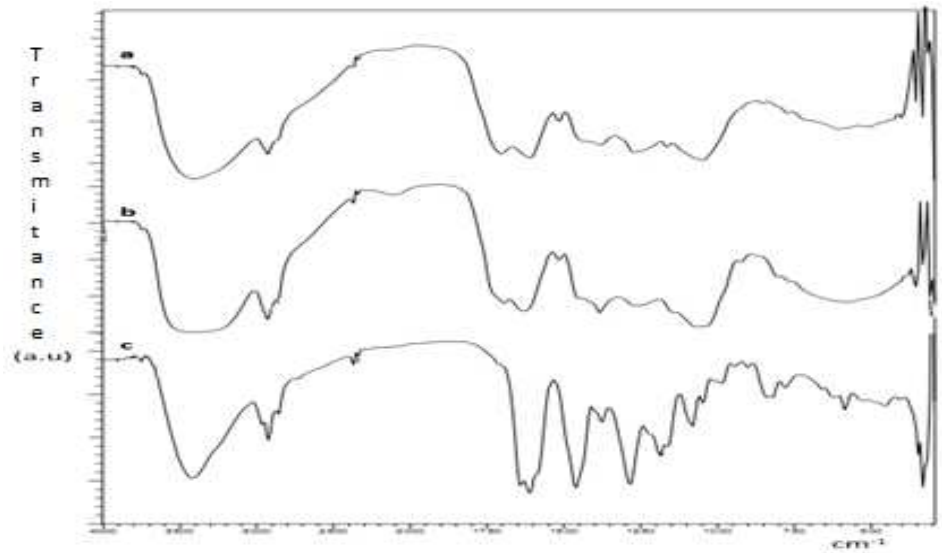


**Figure 1. FTIR Characterization of Ethanol Extracts on Herbal Medicine; a) Majapahit, b ) Pegagan and c) Mangosteen Rind**

The results characterization using infrared spectroscopy (IR) shows any differences of vibration from active compounds. This vibration indicate any different types of active compounds were found in pegagan, majapahit and mangosteen rind. FTIR spectrum profile showed that both ethanol extracts of pegagan, majapahit and mangosteen rind have a vibration hydroxyl groups at wavenumber 3400-3500 $cm^{-1}$ (Figure 1). The vibration for aromatic alkenes at wavenumber of about 1500 $cm^{-1}$ and 1600 $cm^{-1}$. This indicates an estimate that the ethanol extracts of pegagan, majapahit and mangosteen rind have active compounds as phenolic group. The differences vibration of functional groups each ethanol extract of mangosteen rind, pegagan and majapahit can be used as a basis for distinguishing an extract for authentication the herb medicine. This fact is evidence to every herbal medicine must be characterized of FTIR spectrum. Mangosteen rind extract clearly have a different spectrum than Pegagan and majapahit (Figure 1).

**Analysis Discriminant using Principle Component Analysis (PCA) of Ethanol Extract of Pegagan, Majapahit and Mangosteen Rind**

The discriminant process of ethanol extract from herb plant is very important. It has advantage for detect the raw herb material. This research show that ethanol extract of mangosteen rind has an antioxidant activity better than pegagan and majapahit. Therefore, this study will observe the modeling Principle Component Analysis (PCA) to discriminant three types herb medicine. [9] have also used the Near Infrared spectroscopy (NIR) for analysis process and rapid observation of the product Traditional Chinese Medicinal (TCM ).

The results of this study indicate that the data processing using PCA from ethanol extracts of herbs have different. The results also showed that the ethanol extract of mangosteen rind most different than ethanol extract of pegagan and majapahit. Those was seen on PCA results that the distance of mangosteen is very far from pegagan and majapahit (Figure 2). This result can compared with in vitro test which ethanol extract of mangosteen rind has $IC_{50}$ most smaller than ethanol extract of Pegagan and majapahit.

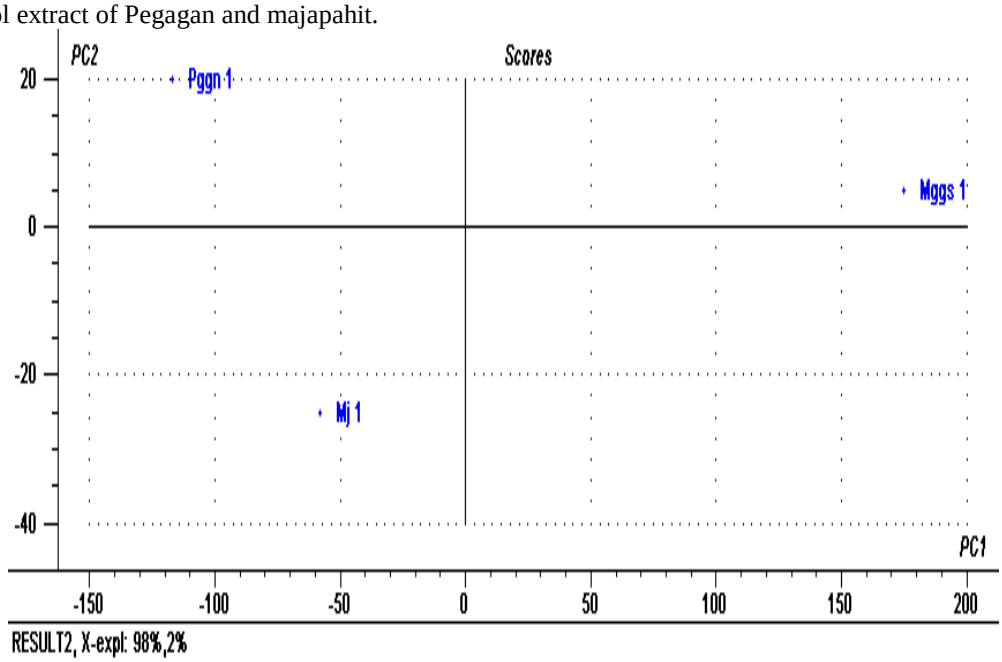


**Figure 2. Results of Data Processing PCA Ethanol Extract Mangosteen Rind, Pegagan and Majapahit**

The discriminant results (Figure 2) shows that the total PC1 and PC2 is 100%. This indicates that the distinction is 100% . Therefore, appropriate data in vitro test from ethanol extract of mangosteen rind has better antioxidant activity and higher total phenol composition. This is reason any different ethanol extract mangosteen rind than ethanol extract of pegagan and majapahit.

PCA processing results show that the outcome from variant residues of ethanol extract of mangosteen rind, pegagan and majapahit less from 3. The results of the ethanol extract of mangosteen rind produce the smaller variants residue (Figure 3). This result shows that FTIR spectrum data used in the discriminant processing has a very significant influence.

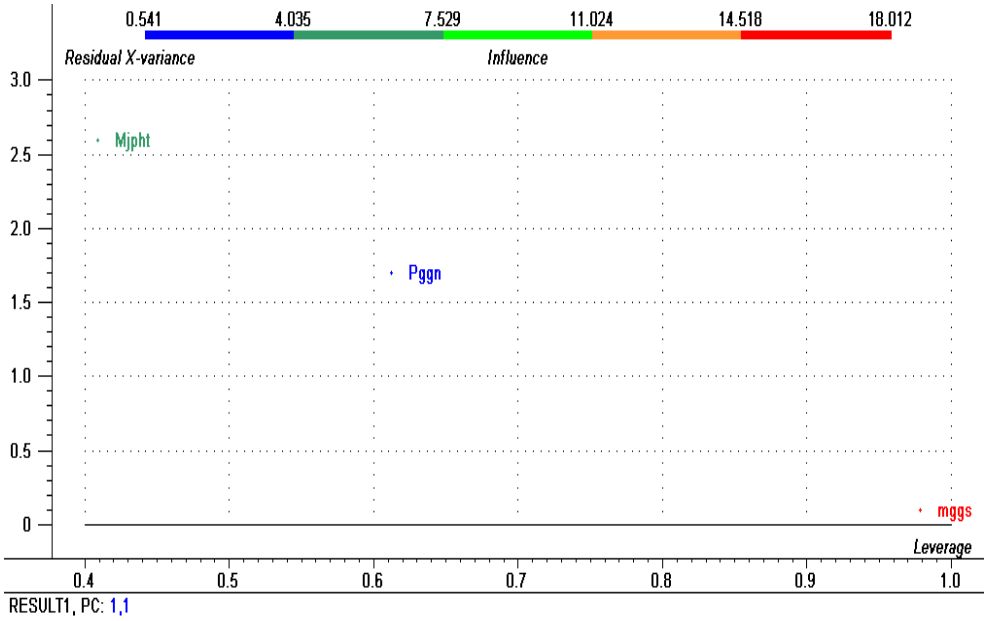


**Figure 3. Residue Analysis of Ethanol Processing PCA Mangosteen Rind Extract, Pegagan and Majapahit**

Figure 3 Shows that the residual variance results showed that no outlayer and this results indicate that the all components in the discriminant process is valid. The figure 3 also shows that the ethanol extract of mangosteen rind has very different characteristics. This fact shown that the different color was produced by the mangosteen rind, Pegagan and majapahit.

**DPPH Inhibition Activity Assay**

The potential of antioxidant activity of ethanol extracts can be known from scavenging activity of free radicals DPPH. This study will compare from activity of ethanol extract of pegagan, majapahit and mangosteen rind. The different of active compound in the extract will give different capabilities in scavenging activity of free radicals DPPH. It can be seen that the ethanol extract of mangosteen rind has higher scavenging activity of free radicals DPPH with regression equation y = 1.083 x + 5.881. The result show the ethanol extract of mangosteen rind has higher antioxidant activity than ethanol extract of pegagan and majapahit (Figure 4).

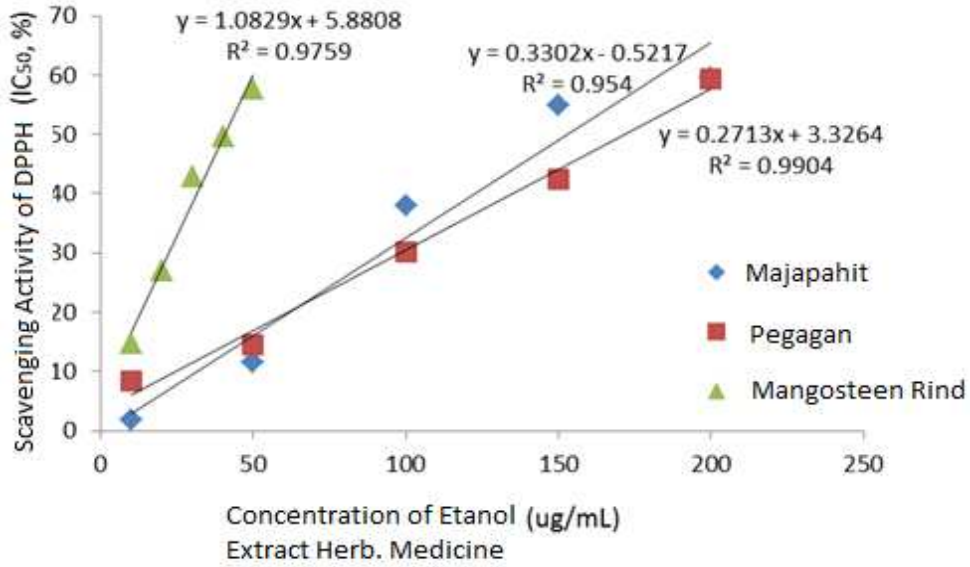


**Figure 4. The Scavenging Activity of DPPH Free Radical with Ethanol Extracts of Pegagan, Majapahit and Mangosteen Rind**

Results of $IC_{50}$ value from ethanol extract of mangosteen rind produce the $IC_{50}$ value smaller than $IC_{50}$ value the ethanol extract of Pegagan and majapahit. The Result of $IC_{50}$ value are 40.1 ug/mL, 172.1 ug/mL and 153 ug/mL respectively. This result shows that the ethanol extract of mangosteen rind has good ability to reduce the free radical of DPPH. The $IC_{50}$ value from mangosteen rind extract is 40.1 ug/mL. It also explains that the ethanol extract of mangosteen rind has ability as an antioxidant better than ethanol extract of pegagan and majapahit.

## CONCLUSION

The results showed that the discriminant process of ethanol extract of mangosteen rind, pegagan, and majapahit using PCA can be used to differentiate each of the extract. The PCA results show that the distance of mangosteen is very far from pegagan and majapahit. In vitro assay, the ethanol extract of mangosteen rind has antioxidant activity better than ethanol extract of pegagan and majapahit. The $IC_{50}$ value from the ethanol extract of mangosteen rind, pegagan and majapahit are 40.1 ug/mL, 172.1 ug/mL and 153 ug/mL respectively.

## REFERENCES

[1] Saifudin, A., Rahayu, V., Teruna, H.Y., Natural Medicinal Materials Standardization, Graha ilmu, Yogyakarta, **2011**
[2] Pasaribu, F., Sitorus, P., dan Bahri, S., *Journal of Pharmaceutics and Pharmacology*, **2012**, vol. 1 (1), 1-8
[3] Putra, I.N.K., *J.Teknol.dan Industri Pangan*, **2010**, XXI, (1), 1-5
[4] Halim, M.R.A.B., Tan, M.S.M.Z., Ismail, S., and Mahmud, R., *International Journal of Pharmacy and Pharmaceutical Science*, **2012**, vol. 4, (3), 606-610
[5] Gautam, A., Kashyap, S.J., Sharma, P.K., Garg, V.K, Visht, S., Kumar, N., *Scholars Research Library*, **2010**, vol. 2, (6): 302-315
[6] Baranowska, I., Srogi, K., Włochowicz, A., Szczepanik, K., *Polish Journal of Environmental Studies*, **2002**, vol. 11 (5), 467-471
[7] Wu, C., Chen, Y., Ouyang K., Taylor, C. and Zhang, Z., Analysis of Chinese herbal medicines by microwave plasma-atomic emission spectrometry (MP-AES), *Agilent Technologies, Inc*, www.agilent.com/chem, **2012**
[8] Kunle, O.F., Egharevba, H.O. and Ahmadu, P.O., *IJBC*, **2012**, vol. 4, (3), 101-112,
[9] Zhang and Su, J., *Acta Pharmaceutica Sinica B*, **2014**, vol. 4, (3), 182-192,
[10] Sim, C.O., Hamdan, M.R., Ismail, Z., and Ahmad, M.,N., *Journal Of Analytica Chimica Acta*, **2004**
[11] Jing, D., Deguang, W., Linfang, H., Shilin, C., and Minjian, Q., *Journal of Medicinal Plants Research*, **2011**, vol. 5, (17), 4001-4008,
[12] Rahayu, R.L.S., and Ahda, M., Conference Proceding ICPCE 2016 : Conference Proceding ICPCE **2016** : Effectiveness of Concentration Ethanol Extraction in Mangosteen Rind (Garcinia Mangostana) and the Correlation Total Phenol Toward Scavenging Activity of Free Radicals DPPH, Waset Publisher, Malaysia, **2016**, 585-588,