Review on the application of chemometrics for the standardization and authentication of *Curcuma xanthorrhiza*

Kusumadewi, A.P., Martien, R., Pramono, S., Setyawan, A.A. and Rohman, A.

1Faculty of Pharmacy, Universitas Gadjah Mada, Yogyakarta 55281, Indonesia.

2Medicinal Plant and Traditional Medicine Research and Development Center, Tawangmangu, Central Java.

3Sekolah Tinggi Ilmu Kesehatan (STIKES) Muhammadiyah, Klaten, Central Java, Indonesia.

4Centre of Excellence Institute for Halal Industry and Systems (PUI-PT IHIS), Universitas Gadjah Mada, Yogyakarta 55281, Indonesia.

Abstract

Temulawak (*Curcuma xanthorrhiza* Roxb.) or Javanese turmeric is one of Indonesia's native medicinal plants and is widely distributed throughout Southeast Asia. Temulawak contains some bioactive compounds having biological activities. The secondary metabolites in temulawak vary widely, depending on the environmental conditions where it grows. Temulawak as a raw material for herbal medicine is often faked with other rhizomes so that the analytical method capable of detecting the adulteration practice of temulawak is needed. The standardization of temulawak is a difficult task because the chemical compounds in temulawak are rather complex. In order to overcome the large and complex data, chemometrics is needed. The purpose of this paper was to highlight the application of chemometrics used during the standardization of temulawak through fingerprinting profile studies. During the literature searching, several databases namely Scopus, Web of Science, Pubmed and Google scholar were explored to get the relevant articles using specific keywords related to the topic. Some chemometrics techniques in combination with several instrumental techniques like spectroscopic and chromatographic methods are successfully used for the characterization and fingerprinting profiling of temulawak. Based on the data synthesized, chemometrics is powerful technique for treating the complex data intended for standardization of temulawak.

1. Introduction

In order to increase the preventive and promotive efforts in the health sector, herbal medicine is one of the people's choices to protect and maintain their health. Temulawak (*Curcuma xanthorrhiza*) is a native Indonesian medicinal plant widely spread to Southeast Asia (Nihayati *et al.*, 2013). Temulawak, known as Javanese turmeric, is a rhizome widely applied as raw material for herbal and food ingredients. The demand for the herbal medicine industry is relatively high with an increase of 5.4% per year. The main chemical contents of *C. xanthorhiza* are xanthorrhizol accounting of 1.48–1.63%, curcuminoids such as curcumin, demethoxycurcumin, bisdemethoxycurcumin accounting of 1–2%, phelandren, camphor, turmerol, cineol, borneol, flavonoids, and sesquiterpenes (Husni, 2016). *C. xanthorrhiza* also contains some essential oils with chemical compounds of β-elemene, β-farnesene, α-curcumene, benzofuran, α-cedrene, epicurzerenone, ar-curcumene, germacrone, aromadendrene, α longipene, trans-caryophiline and curcuphenol (Rafi, Septaningsih and Heryanto, 2018). These compounds are responsible for the yellow to orange color, as well as for the biological activities of temulawak (Itokawa *et al.*, 1985).

Currently, the awareness and public concern in the standardization, authenticity, and quality of herbal medicines has increased significantly, therefore, analytical methods have been developed to perform these tasks (Rohman, Rawar, Sudevi *et al.*, 2020). Herbal medicines have many complex chemical contents characterized by specific markers to differentiate plant species. Their biological activities are the cumulative effects of many chemical compounds (Jia *et al.*, 2017). Some factors contribute to the biological activities such as time harvesting, seasons, plant age, therefore, some
efforts are needed to standardize the herbal raw materials in order to ensure the quality of the herbs (Gopi et al., 2019). Medicinal plants with complex chemical contents, of course, require a special method for quality controls through physico-chemical and molecular biology analyses (Ni et al., 2009). The process of identification and analysis of chemical constituents in medicinal plants can be performed by three approaches namely single component analysis through analysis of specific markers, fingerprinting analysis and metabolomic (Esteki et al., 2018) using some instrumental techniques including molecular spectroscopic and chromatography methods (Mazina et al., 2015). Temulawak is widely applied in herbal and traditional medicine products. Due to its high demand, temulawak is the potential to be substituted or adulterated with other species having a similar appearance such as *Curcuma domestica* (Muttaqin, 2018), therefore, it is very important to standardize temulawak to assure its quality (Windarsih et al., 2021).

The standardization of herbal medicine using fingerprinting profiling and metabolomics resulted in large numbers of responses which make it difficult to handle them. Fortunately, the special statistical package known as chemometrics could resolve this problem. Almost fingerprinting profiling and metabolomic studies used chemometrics for special purposes including pattern recognition and multivariate calibration (Granato et al., 2018). Chemometrics is a combination of mathematical and statistical techniques to process chemical data (Rohman, 2017). Some reviews on the application of chemometrics in herbal standardization include Traditional Chinese Medicines (Razmovski et al., 2010; Bansal et al., 2014; Li et al., 2020). Therefore, the purpose of this paper is to highlight the application of chemometrics used during the standardization of temulawak. In authentication of herbal medicine, the identification of the geographical origin of a medicinal plant including *C. xanthorrhiza* is part of drug analysis and part of quality control in pharmaceutical analysis. Identifying the geographic origin of plant material is a difficult task to do chemically, thus, an application of chemometrics is required to perform these tasks (Xie et al., 2006).

2. Methods

During performing this narrative review, we followed some steps as suggested in several papers reporting the writing of the review articles (Green et al., 2006; Gasparyan et al., 2011; Gregory and Dennis, 2018). The databases used during searching works of literature needed for writing review articles were Web of Science, Scopus, PubMed and Google Scholar. The keywords used for information search are *Curcuma xanthorrhiza* + chemometric OR *Curcuma xanthorrhiza* + standardization OR *Curcuma xanthorrhiza* + geographic origin.

3. Chemometrics

According to the International Chemometrics Society (ICS), the definition of chemometrics is described as “the science of relating chemical measurements made on a chemical system to the property of interest (such as concentration) through the application of mathematical or statistical methods (Rohman and Windarsih., 2020). Chemometrics is a branch of science, which relates the chemical analysis, mathematical or statistical methods (Gemperline, 2006). In chemometrics, some analytical purposes namely quantitative analysis using multivariate calibration, identification or classification using supervised or unsupervised pattern recognition are commonly applied in chemical sciences including authentication and standardization of herbal medicines (Brereton, 2003; Rohman et al., 2014). For example, in pattern recognition using chromatography methods, the samples are grouped according to their measurement (responses) using chromatogram which is the specific character of the analyzed sample (Beebe et al., 1998). The variables used during this task can be retention time, peak area, and peak height. The data were displayed in the form of a matrix consisting of rows and columns written numerically. Each row relates to one object and each column relates to certain features of the object or samples (Massart et al., 1997). Chemometric methods in data analysis are pervasive and important in the decision-making and problem-solving processes. The chemical analysis deals with complex mixtures, compounds, and their properties, which are often very complicated to be analyzed. Therefore, chemometrics is suitable for the analysis of herbal medicines which are typically complex in nature (Rohman, Rawar, Sudevi et al., 2020).

Today with the sophisticated development of statistical software and computers, chemometrics have become the main tool for processing data (Bansal et al., 2014). Several chemometric techniques applied in the standardization and authentication of herbal medicine are data preprocessing such as normalization and derivatization, data exploratory using Principal Component Analysis (PCA), unsupervised pattern recognition using Soft Independent Modeling of Class Analogy (SIMCA) and cluster analysis, supervised pattern recognition such as discriminant analysis and multivariate calibrations such as partial least square regression and principle component regression (Bansal et al., 2014).

In herbal standardization including *C. xanthorrhiza*,

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the chemometrics techniques are applied during fingerprint profiling and metabolomic studies (Bansal et al., 2014; Rohman, Ghazali, Windarsih et al., 2020). While in the authentication studies, chemometrics assisted in determining the origin of herbal medicine, adulteration of high-quality components of herbal medicines with the lower one, or identification of undeclared components in herbal products (Liu et al., 2020). Fingerprint profiling can be obtained from spectroscopic, chromatographic or electrophoretic data. The fingerprint profile must be able to display the similarities and differences in the analyzed samples (Cubero-Leon et al., 2014). The authentication of herbal medicine is a difficult task because many components of medicinal plants are unknown (Bauer, 1998). Fortunately, the chromatography and spectroscopy methods are able to show very strong authentication techniques through fingerprinting profiles. Combining the chemometrics with instrumental responses, the standardization of herbal medicine can be achieved with high precision and accuracy (Gad et al., 2013).

4. Application of chemometrics in standardization of Curcuma xanthorrhiza

Some chemometrics techniques of pattern recognition and multivariate calibrations combined with some instrumental techniques of spectroscopic and chromatographic methods were applied for the standardization of Temulawak. The variables used for chemometrics analysis using spectroscopic methods are absorbance values or ratios at specific wavelengths or wavenumbers, while variables exploited using chromatographic techniques were retention time, peak area, peak height or its ratios (Li et al., 2020). Table 1 compiled some chemometrics methods combined with instrumental techniques for the identification and discrimination of Temulawak, intended for standardization as described in Table 1.

4.1. Principal component analysis

Principal component analysis (PCA) is an exploratory data analysis commonly used for the classification of samples (Irnaewati et al., 2021), and two outputs in PCA commonly reported during classification or clustering are principal components (PCs) and loading plots. PCs are useful to identify any groupings in the data set. In addition, loading plots are shown from coefficients by which the original variables are multiplied in order to get PCs values. Loading plots describe the variables responsible for the separation and or classification of objects (Kim et al., 2010). The identification and discrimination of similar plants, such as turmeric (C. longa), Javanese turmeric (C. xanthorrhiza) and Bangile (Zingiber cassumunar), need to be done to ensure the quality of raw materials used (Rohaeti et al., 2015). Fourier transform Infrared (FTIR) spectroscopy combined with chemometrics can be the method of choice because of the analysis due to its nature as a fingerprint. Visual discrimination of the three species is indicated by the marker bands of FTIR spectra of each species. PCA followed by Canonic Variate Analysis (CVA) using FTIR spectra could classify these plants (Rohaeti et al., 2015).

PCA and discriminant analysis in combination with UV spectroscopy have been applied for the differentiation of four Curcuma species, namely Curcuma xanthorrhiza, C. longa, C. aeruginosa and C. mangga. These four rhizomes are widely used in herbal medicine and dietary supplements. The absorbance values of UV-Vis spectra at the wavelength of 210-500 nm were used as variables during differentiation. UV-Vis spectra were acquired in the interval of 200-800 nm and the standard normal variate was used for preprocessing the spectral data. Using two PCs (PC1 and PC2), PCA could differentiate Curcumas in which PC1 and PC2 were accounting for 79.30% and 12.0%, respectively. In addition, DA using discriminant function 1 (DF1) and discriminant function 2 (DF2) could discriminate four species with an accuracy rate of the correctness of 95.5% (Rafi et al., 2018). PCA is also applied for the differentiation of C. xanthorrhiza, C. aeruginosa, and C. longa using two-dimensional NMR spectra. PC1 and PC2 were accounting for 63.1% and 28.1%, respectively. Based on the identification of metabolites, curcumin and xanthorrhizol are responsible for this differentiation (Wahyuni et al., 2019).

Multivariate analysis of PCA using data set obtained from ³H-NMR spectra clearly discriminated pure and adulterated C. xanthorrhiza with C. aeruginosa as shown in Figure 1. PCA using two PCs showed a clear separation between pure C. xanthorrhiza, pure C. aeruginosa, and adulterated C. xanthorrhiza using several concentration levels of C. aeruginosa. Several original variables used for making the PCA model were reduced to be principal components, which explains the original variables. PC1 and PC2 described 73% of PC1 and 24% of PC2.

Research has been carried out on the existence of adulteration of C. xanthorrhiza with C. domestica, based on the fingerprint profiling by Thin Layer Chromatography (TLC). Fingerprinting profiles of C. xanthorrhiza were obtained from C. xanthorrhiza from Cianjur, Semarang, and East Nusa Tenggara, while the fingerprint profiles of C. domestica were obtained from Cianjur regions. Furthermore, the analysis was carried out by PCA. The results of PCA analysis showed that the
Table 1. The application of several chemometric techniques for the identification and discrimination of C. xanthorrhiza, intended for standardization, authentication and quality controls

| Chemometrics techniques | Methods used | Potency used | Issues | Remark |
|-------------------------|--------------|--------------|--------|--------|
| PLSR                    | FTIR spectroscopy (4000-650 cm⁻¹) | Determination of C. xanthorrhiza by FTIR spectroscopy | Quantitative analysis of curcinoids in C. xanthorrhiza extract could be performed accurately | Lestari et al. (2017) |
| PCA                     | FTIR spectroscopy (4000-650 cm⁻¹) | Determination of C. xanthorrhiza from other Curcuma species for authentication of herbal medicine | These chemometrics using absorbance values at 4000-650 cm⁻¹ could predict the contents of curcumin in C. xanthorrhiza extract | Rohan et al. (2015) |
| PCA                     | NMR spectroscopy (4000-600 cm⁻¹) | Differentiation and quantification of Curcuma species, while PLSR spectra and HPLC combined with these chemometrics could discriminate Curcuma species for authentication issues of herbal medicine | Chemometrics of PLS-DA using 7 principal components (PCs) could classify between authentic and adulterated samples of C. xanthorrhiza | Windarsih et al. (2020) |
| PCA                     | UV-vis (DPPH at 515 nm) | Differentiation of C. xanthorrhiza from Zingiber montanum for authentication studies | I-H-NMR-based metabolite fingerprinting coupled with PCA and OPLS-DA offers an adequate method to assess adulteration practice and to evaluate the authentication of C. xanthorrhiza extracts. | Rohman, Ghazali Windarsih et al. (2020) |
| PCA                     | HPLC         | Differentiation of C. xanthorrhiza for authentication studies | Two-dimensional (2D) NMR spectroscopy could differentiate Curcuma species from different origins | Rohman, Ghazali Windarsih et al. (2020) |
| PCA                     | 1H-NMR-based metabolite fingerprinting coupled with PCA and OPLS-DA | Differentiation of Curcuma species including C. xanthorrhiza for authentication studies | Curcuma species based on metabolites contained in Curcuma species with a success rate of 95.5% | Windarsih et al. (2020) |
| PCA                     | UV-vis spectroscopy (200-800 nm) | Differentiation of Curcuma species including C. xanthorrhiza for authentication studies | Da offered a better classification of C. xanthorrhiza with a success rate of 95.5% | Windarsih et al. (2020) |
fingerprints of *C. xanthorrhiza* and *C. domestica* were in different quadrants. However, analysis of instant curcuma samples showed that the samples were in the quadrant between *C. xanthorrhiza* and *C. domestica* (Muttaqin et al., 2018). PCA was also successfully used for the classification of other Curcuma species intended for hindering the adulteration practice (Windarsih et al., 2019).

\[ \text{Figure 1. The score plots of principal component analysis for classification of pure } C. \text{xanthorrhiza, pure } C. \text{aeruginosa, and adulterated } C. \text{xanthorrhiza. The output was obtained using SIMCA 14.0 software (Sartorius, Malmo, Sweden). Source: Rohman, Wijayanti, Windarsih et al. (2020).} \]

### 4.2 Discriminant analysis

Discriminant analysis (DA) is one of the supervised pattern recognitions commonly used for the discrimination or classification of objects/samples into several groups (Rohman and Putri, 2019). DA using algorithm of orthogonal projections to latent structures (OPLS) has been applied for the authentication of *C. xanthorrhiza* with *C. aeruginosa* using variables of $^1$H-NMR spectra. OPLS-DA was successfully applied for the classification of pure and adulterated *C. xanthorrhiza* with higher R2X (0.965), R2Y (0.958), and Q2(cum) (0.93) as shown in Figure 1 (Rohman, Wijayanti, Windarsih et al., 2020). Authentication and discrimination studies have also been conducted to differentiate the fingerprints of *C. xanthorrhiza* and *C. longa* based on curcuminoi d levels using HPLC assisted with chemometrics of DA. This combination can separate *C. xanthorrhiza* and *C. longa* species (Rafi et al., 2015). In addition, the combination of 1H-NMR and chemometric methods are promising for the authentication of medicinal plants (Windarsih et al., 2021). $^1$H-NMR spectroscopy and chemometrics have been applied to authenticate *C. xanthorrhiza* adulterated with *Zingiber cassumunar*. Partial least square-discriminant analysis (PLS-DA) using 7 main components (PCs) was successfully classified the original sample and the adulterated *C. xanthorrhiza* with values of R2X (0.988), R2Y (0.998), and Q2 (0.993). The chemometrics of PCA and PLS-DA allows for the discrimination of pure *C. xanthorrhiza* and *C. xanthorrhiza* adulterated with *Z. cassumunar* (Wijayanti et al., 2019).

### 4.3 Multivariate calibrations

Multivariate calibration is one of the quantitative tools for prediction of analyte(s) of interest in herbal medicine like curcumin in Temulawak using several variables. Partial least square regression (PLSR) and principle component regression (PCR) are the most applied techniques (Keithley et al., 2009). PLSR using absorbance values of FTIR spectra at 4000-650 cm$^{-1}$ has been used to predict the levels of curcumin (C), demethoxycurcumin (DM) and total curcuminoid (TC) in *C. xanthorrhiza* intended for the standardization. The actual contents of curcuminoi d in the ethanolic extract of *C. xanthorrhiza* were previously determined using HPLC with a PDA detector. With PLSR, the R$^2$ values of the calibration model for CUR, DMCUR and TCUR were > 0.99. The levels of curcuminoi d determined using FTIR spectroscopy-PLSR were not statistically significant compared with the HPLC method based on an independent sample t-test (P > 0.05) (Lestari et al., 2017).

The combination of FTIR spectra-PLSR was also successfully applied for the prediction of the levels of curcumin in curcuma in *C. longa* and *C. xanthorrhiza*. The actual levels of curcumin were determined using HPLC. PLSR using absorbance values at wavenumbers of 2000-950 cm$^{-1}$ was suitable for the prediction of curcumin. The R$^2$ values for the correlation between actual values and FTIR predicted values of curcumin were 0.96 and 0.99 with RMSEC values of 0.299 and 0.089 in *C. longa* and *C. xanthorrhiza*, respectively. High R$^2$ values and low RMSEC values indicated high accuracy and precision of the analytical method (Rohman et al., 2015).

### 5. Conclusion

Several chemometrics techniques either pattern recognition (supervised such as discriminant analysis and unsupervised like principal component analysis) or multivariate calibrations like partial least square using variables generated from several instrumental techniques like spectroscopic and chromatographic methods are successfully used for characterization and fingerprinting profiling of herbal medicines including Temulawak intended for the authentication, quality control and standardization of herbal medicine. Based on the data synthesized, chemometrics is a powerful and meaningful technique for treating the complex data intended for the standardization and authentication of herbal medicines such as Javanese Turmeric.
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