Case Studies in Chemical and Environmental Engineering 10 (2024) 100994

Contents lists available at ScienceDirect

Case Studies in Chemical and Environmental Engineering

journal homepage: www.sciencedirect.com/journal/case-studies-in-chemical-and-environmental-engineering

Case Report

Moringa oleifera seed oils: Physico-chemical characterization and its authentication using FTIR spectroscopy and chemometrics

Irnawati [a,b], Abdul Rohman [c,d,*], Yamin [b,c], Nurrulhidayah Ahmad Fadzillah [e], Aida Azrina Azmi [f], Nurlatifah [g], Anjar Windarsih [h], Ratna Asmah Susidarti [c], Ruslin [b]

[a] *Universitas Gadjah Mada, Yogyakarta, Indonesia*
[b] *Faculty of Pharmacy, Universitas Halu Oleo, Kendari, Indonesia*
[c] *Department of Pharmaceutical Chemistry, Faculty of Pharmacy, Universitas Gadjah Mada, Yogyakarta, Indonesia*
[d] *Center of Excellence, Institute of Halal Industry and Systems (IHIS), Universitas Gadjah Mada, Yogyakarta, 55281, Indonesia*
[e] *International Institute for Halal Research and Training (INHART), International Islamic University Malaysia, Kuala Lumpur, Malaysia*
[f] *Halal Products Research Institute, University Putra Malaysia, Serdang, Malaysia*
[g] *Animal Science Learning Center, Universitas Gadjah Mada, Yogyakarta, Indonesia*
[h] *Research Center for Food Technology and Processing (PRTPP), National Research and Innovation Agency (BRIN), Yogyakarta, 55861, Indonesia*

ARTICLE INFO

Keywords:
Moringa oleifera seed oil
Chemometrics
Authentication analysis
Soybean oil
Physico-chemical properties

ABSTRACT

Study on fatty acid compositions and authentication of *Moringa oleifera* seed oil (MOSO) is essential. MOSO from different regions had acid values of 0.32 ± 0.01 mg KOH/g, saponification values of 182.50 ± 5.95 mg KOH/g, iodine values of 78.30 ± 4.24 g I_2/100 g, and peroxide values of 1.12 ± 0.02 meq O_2/kg MOSO. The dominant fatty acids of MOSO were oleic acid (68.31–76.89 %) and palmitic acid (6.17–8.27 %), respectively. The chemometrics of partial least square-discriminant analysis (PLS-DA) could classify of MOSO using fatty acid compositions as variable into two distinct groups using two discriminant components in which the first and second components could describe 62.5 % and 18.7 %, respectively. Partial least square (PLS) could predict soybean oil levels as adulterant at combined wavenumbers region of 2935-2830 and 1800-710 cm^{-1}. The coefficient of determination (R^2) in calibration and validation models were of 0.9971 and 0.9961, with root mean square error of calibration (RMSEC) and root mean square error of prediction (RMSEP) of 1.67 % and 1.93 %, respectively. In summary, MOSO contains good physico-chemical properties including fatty acid compositions which are beneficial for its application in pharmaceutical, nutraceutical, and cosmetic products in the future. We concluded that the FTIR spectroscopy and chemometrics are promising tools for the authentication study and quality control of MOSO.

1. Introduction

Moringa oleifera, also known as *miracle tree*, belonging to the Moringaceae family has been used for thousands of years by numerous civilizations including Indian, Greek, and Egyptian, and it is also used as a traditional herbal medicine in Ayurveda, Unani, and Siddha medicine systems [1]. The use of *M. oleifera* plants has been extensively studied throughout several domains of functional food and medicine, due to its low toxicity with minimum side effects [2]. The biological effects of *M. oleifera* are influenced by numerous factors, such as the phytochemicals component along with extraction methods, purification techniques, and structural diversity [3,4]. In addition, the seed of *M. oleifera* also contains edible oils with valuable phytochemicals components having the pharmacological activities toward human health [5] such as antioxidant compounds [6], phenolics contents [7] as well as unsaturated fatty acids of oleic (C18:1) and linoleic acids (C18:2) [8]. For this reason, the characterization of edible oils extracted from plant sources is needed to ascertain the physico-chemical properties of the corresponding oils [9,10].

Some extraction methods have been developed including conventional techniques such as direct pressing, solid-liquid extractions (maceration, Bligh-Dyer and Soxhlet extraction) [11] and non-conventional methods like ultrasonic assisted extraction (UAE) assisted by experimental designs [12], microwave-assisted extraction (MAE) [13], and supercritical CO_2 extraction assisted by response surface methodology [14]. The different extraction techniques of edible fats

* Corresponding author. Department of Pharmaceutical Chemistry, Faculty of Pharmacy, Universitas Gadjah Mada, Yogyakarta, 55281, Indonesia.
E-mail address: abdul_kimfar@ugm.ac.id (A. Rohman).

https://doi.org/10.1016/j.cscee.2024.100994
Received 13 June 2024; Received in revised form 23 October 2024; Accepted 29 October 2024
Available online 30 October 2024

and oils could provide the different results in terms of physico-chemical properties, phytochemical compositions and biological activities due to the different types and concentrations of chemical compounds extracted [11]. In Indonesian market, *M. oleifera* seed oil (MOSO) is sold in the range of 15–20 US$, while the common vegetable oils like palm, corn and soybean oils are available in market with price of 2–4 US$, therefore MOSO is potential to be adulterated with these vegetable oils by unethical businessman to gain the economical profit. Indeed, the adulteration practice in fats and oils industry is serious matters not only for economic reasons but also for health issues in which the foreign materials used as adulterant could be allergenic to certain people, therefore the research on the authentication of high price oils such MOSO is emerging issue by food scientists [15]. In addition, Santos et al. have stated that vegetable oils like MOSO are renewable raw materials used widely. MOSO that could be adulterated with other vegetable oils has similar characteristics, such as olive and buriti oils [16].

Numerous analytical methods applying some physico-chemical constants and instrumental analyses have been explored and reported for the authentication of expensive and high-quality edible oils. The sophisticated instruments such as near infrared, FTIR, Raman, and NMR spectrophotometers [17], chromatograph hyphenated with mass spectrometer like GC-MS and LC-MS mainly through metabolomics approach [18], thermal analyses like differential scanning calorimetry [19] and some rapid methods like electronic nose and electronic tongue [20] have been developed and validated for the authentication of fats and oils. For routine analysis, FTIR spectroscopy combined with chemometrics or multivariate data analysis could be the ideal method for the authentication of edible fats and oils. The combination of FTIR spectroscopy and chemometrics offers rapid and accurate method with minimum or without sample preparation and simple instrument operation [21] and is successfully employed for the authentication of olive oil [22], avocado oil [23], and red fruit oil [24]. Using detail literature analysis, the research on the authentication of MOSO applying different analytical methods is very limited.

To the best of our knowledge, research on the exploration of physico-chemical properties of MOSO obtained from different regions in Indonesia remains limited. In addition, there is a few studies reported the use of vibrational spectroscopy such as FTIR spectroscopy coupled with chemometrics of partial least squares regression (PLSR) and principal component regression (PCR) on the analysis of adulterants present in MOSO. Therefore, this study highlighted the characterization of MOSO obtained from different regions through determining some parameters related to edible oils such as the physico-chemical properties and fatty acid compositions of MOSO. This information showed the beneficial constituents of MOSO for further applications in pharmaceutical, nutraceutical, as well as cosmetic products. Then, the second objective was to develop a fast and effective authentication analysis of MOSO from potential adulterants using FTIR spectroscopy and chemometrics which can be applied as a method for rapid and reliable analytical method for quality control of MOSO.

2. Materials and methods

2.1. Materials

The seeds of *Moringa oleifera* was taken from some regions of Southeast Sulawesi (Kendari), Yogyakarta and Central Java (Demak and Pati), Indonesia. The authentication analysis of materials or samples used (*M. oleifera*) was performed in the Laboratory of Pharmacognosy, Department of Pharmaceutical Biology, Faculty of Pharmacy, Yogyakarta Indonesia. Some common vegetable oils which are potential to be used as adulterants to MOSO namely corn, palm, canola, sunflower, soybean, mustard, avocado, olive, and coconut oils were purchased from several markets and supermarkets in Yogyakarta. The reagents and solvents used for physico-chemical characterization and fatty acid analyses were of pro-analytical grade.

2.2. Preparation of MOSO

Preparation of MOSO was carried out according to Mai et al. [25]. Seeds obtained from the mature pods were subjected to powdering and the obtained powders were macerated with hexane (1: 8) for 2 × 24 hours with automatic shaking for 45 min in each day. The mixture is filtered using vacuum filter, and the solution was evaporated at 50 °C using a rotary evaporator (Rotavapor®, Buchi) to obtain MOSO. These oils were then used for chemical analyses, fatty acid composition and authentication analysis using FTIR analysis.

2.3. Chemical analyses of MOSO

Some constants which are related to the composition and quality assessment of MOSO were carried out based on procedure in the American Oil Chemists' Society (AOCS) methods. MOSO samples were subjected for chemical analyses including acid value (Cd 3a–63), saponification (Cd 3–25), iodine value (Cd 1d-92), peroxide value (Cd 8–53), and anisidine value (Cd 18–90).

2.4. Analysis of fatty acid composition

Fatty acid composition of MOSO from different locations were determined using gas chromatograph equipped with flame ionization detector (GC-MS) according to our previous paper [26]. MOSO samples were subjected to derivatization procedure (base-catalyzed followed by the methanolic BF_3 method) to provide fatty acid methyl esters (FAMEs) which are suitable to be analyzed using GC since FAMEs are volatile enough and stable to heat. A-50 μL MOSO from different origins were added with 1.5 mL of MeOH–KOH, heated at 60 °C for 10 min, cooled at room temperature and then added 2.0 mL BF_3–CH_3OH. The mixtures were heated again under the same condition, when cooled, 1 mL of heptane was added, shacked and centrifuge at 3000 rpm for 1 min. Finally, the FAMEs in heptane layer were subjected to GC (Agilent Technologies, 7890B) and flame ionization detector (FID). GC was equipped with a capillary column of DB-Fast-FAME (30 m × 250 × 0.25 μm). The temperatures of the injection inlet and FID were 250 °C and 280 °C, respectively. The initial temperature of the column was set at 60 °C for 1 min and ramped to 150 °C (30 °C/min), hold in 1 min and increased to 200 °C (3 °C/min), hold in 5 min, and finally increased to 225 °C (0 °C/min) and hold for 3 min. The injection volume was 1.0 μL using Split mode (10: 1). Carrier gas of helium (H_2) with ultra-high purity (UHP) 99,999 % was delivered at 1.0 mL/min. For MS condition, the mass ranges were 30–500 amu. The temperatures of ion sources and quadrupole were of 230 °C and 150 °C, respectively. The confirmation of fatty acids was carried out by comparing the retention times of fatty acids in MOSO samples to those in 37 mix standard of fatty acid methyl esters (FAMEs) from Sigma (USA). The oleic acid as major fatty acid in MOSO was identified at retention time of 17 min. In addition, the fatty acids were also confirmed from mass spectra obtained from GC-MS measurement. Quantification of fatty acids were performed using internal normalization technique (area normalization) as in Rohman and Che Man [27].

2.5. Authentication analysis of MOSO using FTIR spectroscopy and chemometrics

The authentication analysis of MOSO from oil adulterants was carried out according to Rohman et al. [28]. The procedure include: (1) preparation of calibration and validation samples by mixing MOSO and soybean oil (Sy-O) as adulterant at concentration ranges of 1–50 % Sy-O in MOSO; (2) FTIR spectral acquisition using ATR-FTIR spectrophotometer from Thermo Scientific Nicolet iS10 (Madison, WI) equipped with ZnSe crystal and OMNIC software for spectral treatments. The scanning of FTIR spectra was carried out in mid infrared region (4000–600 cm^{-1}) with scanning number of 32 and resolution of 8 cm^{-1};

(3) optimization and quantitative modelling of MOSO adulterated with Sy-O by assessing some parameters including the spectral treatments (normal and derivatives), the wavenumbers region which provide the differentiation between MOSO and Sy-O, and the types of multivariate calibrations. Spectral derivation was carried out using tools provided by TQ analyst software.

2.6. Data analysis

The data generated from determination of the constant numbers (acid number, saponification number, iodine number and peroxide value) and fatty acid compositions were expressed as mean ± standard deviation. The statistical test of ANOVA was applied using Minitab software. Tukey's post hoc test was used to evaluate statistical significance ($p < 0.05$). The Data obtained from the authentication analysis of MOSO from Sy-O were subjected to chemometrics of multivariate calibrations (PLSR and PCR) and pattern recognition of PLS-DA. All chemometrics analysis was carried out using TQ Analyst software included in FTIR spectrophotometer used for FTIR spectral scanning.

3. Result and discussion

3.1. Physico-chemical properties and fatty acid compositions of MOSO

Edible fats and oils including MOSO are basically triacyclglycerols (TAG), in which three fatty acids present in MOSO were esterified with glycerol. Fatty acid compositions are fingerprint in nature in which there are no edible fats and oils having the same compositions of fatty acids in terms of types and the concentrations of each fatty acids, therefore FAs composition could be used for the characterization of edible fats and oils [29]. The standard method for analysis of FAs composition is gas chromatography equipped with flame ionization detector or mass spectrometer detector (GC-MS). In this study, GC-MS has been successfully applied for analysis of FAs in MOSO with high sensitivity and specificity. Fig. 1 exhibited the total ion chromatogram (TIC) of fatty acid methyl esters (FAMEs) standard and FAMEs in MOSO.

Good separation and efficiency were achieved using the optimized GC-MS condition. Table 1 compiled FAs composition of MOSO obtained from several regions in Southeast Sulawesi and central Java. The dominant fatty acids composed MOSO were oleic acid (C18:1) and palmitic acid (C16:0) accounting of 68.31–76.89 % and 6.17–8.27 %, respectively. These results were in agreement with those reported by Özcan [30] and Ali et al. [31] in which both C18:1 and C16:0 are dominant fatty acids composed MOSO obtained from Turkey and Egypt, respectively. In addition, the samples of MOSO from different regions were also characterized by some physico-chemical constants namely

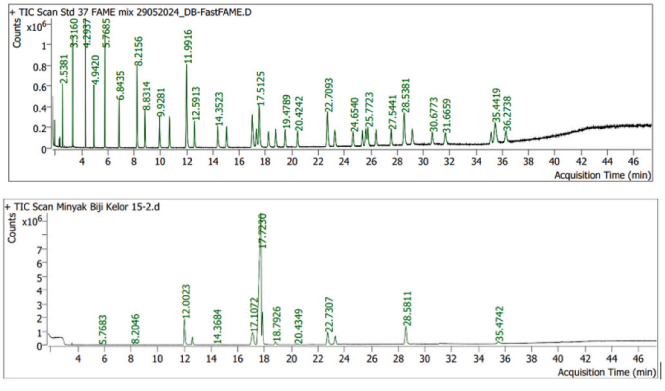

Fig. 1. The total ion chromatogram (TIC) obtained during the separation of standard of fatty acid methyl esters (FAMEs) and FAMEs in *Moringa oleifera* seed oils MOSO using gas chromatography-mass spectrometry (GC-MS). For GC-MS conditions, see Section of Methods.

acid values of 0.32 ± 0.01 mg KOH/g, saponification values of 182.50 ± 5.95 mg KOH/g, iodine values of 78.30 ± 4.24 g I_2/100 g, and peroxide values of 1.12 ± 0.02 meq O_2/kg MOSO. These results were similar to those reported by Ogunsina et al. [32]. The results of this study were also comparable with the results from MOSO obtained from cold press extraction. Gharsallah et al. [33] reported that MOSO from cold pressed extraction had an acid value of 1.5 ± 0.21 mg KOH/g oil, saponification value of 168.3 ± 0.45 mg KOH/g oil, iodine value of 67.42 ± 0.21 g I_2/100 g oil, and peroxide value of 7.5 ± 0.03 meq O_2/kg oil. Our study revealed that the obtained MOSO in our study had a lower acid value and peroxide value which are preferred for better quality of MOSO. The differences in chemical properties of the MOSO are influenced by the oil extraction method and origin of Moringa seed [34].

Fatty acid compositions were further used as variables for classification of MOSO coming from the different regions using the chemometrics of pattern recognitions of principal component analysis (PCA) and of partial least square-discriminant analysis (PLS-DA). Fig. 2 showed the pattern recognition of PCA and PLS-DA in which PLS-DA could better separation of MOSOs than PCA. PCA works by reducing the original variables into a number of principal components (PC) representing the variation of original variables.

In this study, PCA using the first two PC could represent 73.8 % and 18.3 % variation from PC1 and PC2, respectively. However, PCA could not separate between group 1 and group 2 of MOSO. It indicated that PCA could not well differentiate MSO using the fatty acid compositions as the variables. It could happen because PCA is an unsupervised pattern recognition, where only focus on the variables reduction to find differences and similarities of samples. As an unsupervised technique, PCA has limitations such as it focuses solely on explaining the variance in the data without considering any class labels. This can lead to difficulties in distinguishing between classes, especially if the variance within classes is high [35]. Therefore, further analysis using other pattern recognition techniques of supervised pattern recognition technique, such as PLS-DA was performed. In this study, PLS-DA using fatty acid compositions as variables could clearly classify MOSO obtained from different origins into two groups, that is group 1 and group 2, in which the first and second components of PLS-DA could describe 62.5 % and 18.7 %, respectively. It means that in group 1, MOSO obtained from Kolaka, Bone, Pati, Wakatobi, Konawe, Buton, Muna, and South Konawe had a similar property in term of fatty acid compositions. Meanwhile, group 2 indicates that MOSO from North Buton, Kendari, South Buton, West Muna, Bau-Bau, Central Buton, and East Kolaka demonstrated similar fatty acid compositions. PLS-DA is a supervised pattern recognition that maximizes variations using latent variables instead of principal components. PLS-DA will search the optimum number of latent variables to obtain the best predictive power which can better distinguish samples [36]. Moreover, PLS-DA incorporates class information, making it more effective for classification tasks. It provides components that are more aligned with class separability, enhancing interpretability regarding the relationship between predictors and classes [35]. In addition, the discrimination result obtained from PLS-DA was evaluated using a cross-validation technique to warrant the performance of PLS-DA [37].

Previously, PCA and PLS-DA has been widely used for classification of oils. Previous research reported the good performance of PLS-DA for classification of five different edible oils including soybean oil, peanut oil, camellia oil, corn oil, and sunflower seed oils. The PLS-DA using FTIR spectra could successfully classified those five different oils with 100 % correct classification rate [38]. Another study reported that adulteration of patchouli oil with gurjun balsam oil (GBO) could be successfully detected using FTIR spectroscopy and PLS-DA. The best separation of pure patchouli oil and those adulterated with GBO was obtained using the original FTIR spectrum of wavenumber range 1800-600 cm^{-1} [39].

Table 1
Fatty acid compositions of Moringa oleifera seed oil (MOSO) obtained from several regions in Southeast Sulawesi and central Java as determined using GC-MS.

Moringa oleifera seed oils	Fatty Acid Composition (%)													
	C12:0	C14:0	C16:0	C16:1	C17:0	C18:0	C18:1	C18:2	C18:3	C20:0	C20:1	C22:0	C22:1	C24:0
Wakatobi	0.011 ± 0.000^{bc}	0.064 ± 0.004^{f}	7.942 ± 0.016^{b}	1.422 ± 0.020^{de}	0.031 ± 0.053^{ab}	5.424 ± 0.041^{de}	70.801 ± 1.408^{ef}	0.772 ± 0.007^{cd}	0.056 ± 0.000^{g}	3.451 ± 0.019^{bc}	2.534 ± 0.065^{bcd}	6.232 ± 0.105^{cd}	nd	0.837 ± 0.032^{a}
West Muna	0.007 ± 0.000^{bc}	0.113 ± 0.005^{bc}	7.459 ± 0.054^{cd}	1.508 ± 0.015^{d}	0.065 ± 0.004^{ab}	3.726 ± 0.116^{g}	73.930 ± 1.383^{bcde}	0.927 ± 0.012^{a}	0.145 ± 0.005^{a}	2.481 ± 0.040^{fg}	2.476 ± 0.046^{cd}	5.392 ± 0.076^{f}	nd	0.889 ± 0.053^{a}
South Buton	nd	0.094 ± 0.006^{de}	6.124 ± 0.046^{h}	1.411 ± 0.010^{de}	0.000 ± 0.000^{b}	3.683 ± 0.044^{g}	75.637 ± 1.450^{abc}	0.676 ± 0.008^{fg}	0.072 ± 0.000^{f}	2.436 ± 0.034^{g}	2.121 ± 0.085^{e}	6.358 ± 0.128^{bc}	nd	0.688 ± 0.033^{abc}
Kendari	nd	0.127 ± 0.006^{b}	7.368 ± 0.157^{cd}	1.891 ± 0.083^{a}	0.025 ± 0.043^{ab}	6.304 ± 0.077^{ab}	72.569 ± 1.400^{cdef}	0.785 ± 0.009^{bcd}	0.145 ± 0.000^{a}	3.399 ± 0.071^{bc}	1.812 ± 0.048^{f}	4.349 ± 0.123^{g}	nd	0.658 ± 0.022^{abc}
East Kolaka	nd	0.053 ± 0.000^{f}	7.173 ± 0.150^{de}	1.171 ± 0.020^{gh}	0.000 ± 0.000^{b}	3.547 ± 0.071^{g}	75.757 ± 1.014^{abc}	0.746 ± 0.010^{de}	0.058 ± 0.000^{g}	2.305 ± 0.033^{g}	2.355 ± 0.080^{d}	5.079 ± 0.141^{f}	nd	0.766 ± 0.298^{ab}
Buton	nd	0.113 ± 0.005^{bc}	7.715 ± 0.052^{bc}	1.068 ± 0.013^{hi}	0.024 ± 0.028^{ab}	6.012 ± 0.130^{bc}	71.990 ± 1.158^{def}	0.779 ± 0.010^{cd}	0.133 ± 0.000^{b}	3.455 ± 0.044^{bc}	2.414 ± 0.241^{d}	5.468 ± 0.061^{ef}	nd	0.859 ± 0.034^{a}
North Buton	0.225 ± 0.015^{a}	0.632 ± 0.016^{a}	8.570 ± 0.289^{a}	0.701 ± 0.019^{j}	0.000 ± 0.000^{b}	4.774 ± 0.096^{f}	72.009 ± 0.514^{def}	0.773 ± 0.031^{cd}	0.085 ± 0.000^{e}	2.673 ± 0.031^{ef}	1.825 ± 0.014^{f}	5.080 ± 0.060^{f}	nd	0.196 ± 0.178^{c}
Konawe	nd	0.129 ± 0.010^{b}	7.139 ± 0.081^{de}	1.045 ± 0.013^{i}	0.000 ± 0.000^{b}	5.668 ± 0.127^{cd}	72.434 ± 0.290^{cdef}	0.816 ± 0.014^{bc}	0.050 ± 0.000^{g}	3.293 ± 0.070^{cd}	2.714 ± 0.000^{b}	6.328 ± 0.228^{bc}	nd	0.709 ± 0.043^{abc}
Bau-Bau	nd	0.058 ± 0.000^{f}	6.834 ± 0.105^{ef}	1.460 ± 0.053^{de}	0.000 ± 0.000^{b}	5.240 ± 0.092e	77.860 ± 0.736^{a}	0.613 ± 0.014^{h}	0.000 ± 0.000^{h}	2.755 ± 0.075^{e}	1.325 ± 0.051^{g}	4.450 ± 0.275^{g}	0.000 ± 0.000^{f}	0.228 ± 0.395^{bc}
Kolaka	0.014 ± 0.000^{b}	0.114 ± 0.000^{bc}	6.750 ± 0.101^{efg}	1.794 ± 0.032^{ab}	0.083 ± 0.004^{a}	6.525 ± 0.099^{a}	69.344 ± 0.931^{f}	0.943 ± 0.025^{a}	0.137 ± 0.000^{b}	4.433 ± 0.059^{a}	3.321 ± 0.956^{a}	5.864 ± 0.097^{de}	0.107 ± 0.006^{a}	1.184 ± 0.031^{a}
Central Buton	nd	0.054 ± 0.000^{f}	7.375 ± 0.259^{cd}	1.353 ± 0.045^{ef}	0.000 ± 0.000^{b}	4.546 ± 0.124^{f}	75.129 ± 0.547^{abcd}	0.607 ± 0.012^{h}	0.000 ± 0.000^{h}	2.745 ± 0.137^{e}	2.136 ± 0.015^{e}	5.068 ± 0.133^{f}	0.000 ± 0.000^{f}	0.705 ± 0.019^{abc}
Muna	nd	0.104 ± 0.000^{cd}	6.353 ± 0.040^{gh}	1.248 ± 0.016^{fg}	0.043 ± 0.042^{ab}	5.348 ± 0.123^{de}	76.167 ± 1.024^{ab}	0.761 ± 0.020^{de}	0.101 ± 0.000^{d}	3.158 ± 0.050^{d}	2.469 ± 0.146^{cd}	6.107 ± 0.240^{cd}	0.051 ± 0.000^{d}	0.762 ± 0.010^{ab}
South Konawe	0.008 ± 0.000^{bc}	0.123 ± 0.005^{b}	8.115 ± 0.132^{b}	1.367 ± 0.026^{e}	0.024 ± 0.042^{ab}	3.811 ± 0.077^{g}	77.305 ± 1.139^{a}	0.714 ± 0.014^{ef}	0.098 ± 0.000^{d}	2.504 ± 0.080^{fg}	2.634 ± 0.009^{bc}	6.678 ± 0.148^{b}	0.058 ± 0.000^{c}	0.725 ± 0.019^{abc}
Pati	nd	0.083 ± 0.000^{e}	6.599 ± 0.160^{fg}	1.736 ± 0.021^{bc}	0.060 ± 0.001^{a}b	5.581 ± 0.086^{de}	71.166 ± 1.224^{ef}	0.654 ± 0.024^{gh}	0.112 ± 0.000^{c}	3.564 ± 0.126^{b}	2.501 ± 0.061^{cd}	7.394 ± 0.065^{a}	0.089 ± 0.000^{b}	0.748 ± 0.07^{3ab}
Bone	0.008 ± 0.000^{bc}	0.120 ± 0.000^{bc}	6.601 ± 0.163fg	1.627 ± 0.067^{c}	0.080 ± 0.001a	6.631 ± 0.306^{a}	69.385 ± 1.489^{f}	0.835 ± 0.033^{b}	0.151 ± 0.009^{a}	4.405 ± 0.045^{a}	2.433 ± 0.042^{d}	6.419 ± 0.091^{bc}	0.029 ± 0.000^{e}	0.751 ± 0.548^{ab}

Mean with different lowercase letters within a column in each origin are significantly different ($p<0.05$) after applying a one-way ANOVA and Tukey's post hoc test. Value are mean ± SD of triplicate. nd = not detected with limit of detection of 0.001 %.

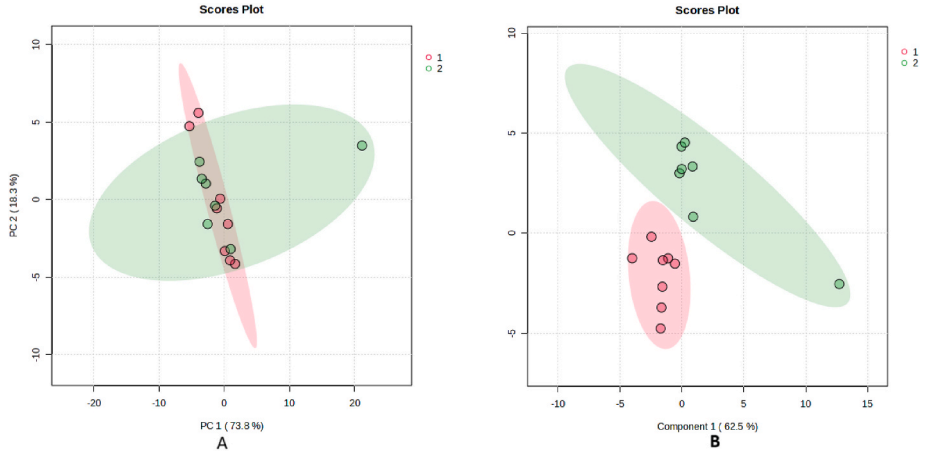

Fig. 2. Principal component analysis (PCA) [A] and partial least square-discriminant analysis (PLS-DA) [B] of *Moringa oleifera* seed oil (MOSO) using fatty acid compositions as variables. (Group 1: Kolaka, Bone, Pati, Wakatobi, Konawe, Buton, Muna, South Konawe; Group 2: North Buton, Kendari, South Buton, West Muna, Bau-Bau, Central Buton, East Kolaka).

3.2. Authentication analysis of MOSO from soybean oil using FTIR spectra and chemometrics

MOSO has high priced values in the Indonesian oil market and it is subjected to adulteration with low price oils such as soybean oil (Sy-O). The quantitative measurement of Sy-O in Moringa seed oil (MOSO) was carried out using multivariate calibration of partial least squares calibration (PLSR) and principal component regression (PCR). The power of PLSR for modelling the actual values and FTIR predicted values was based on its capacity to acquire the spectral information from certain spectral regions and to create a regression equation [40]. The FTIR spectral regions where changes were detected between MOSO and Sy-O (3010-2830 and 1800-650 cm^{-1}) (Fig. 3) were employed to create PLSR models. In this region, the statistical results including the coefficient of determination (R^2) either in calibration or validation models, root mean square error of calibration (RMSEC), and root mean square error of calibration or validation (RMSEP) were compiled in Table 2.

The selection of wavenumbers regions offering the best prediction model is the important steps during chemometrics modelling. It is not always possible to obtain a good multivariate prediction model by using the entire spectral region of the vibrational spectra. Some wavelengths do not contain the necessary information, which may interfere with the establishment of quantitative model. Selecting wavelengths that are highly related to target sample characteristics could contribute to the reduction of redundancy [41]. In this study, the full range and selected range wavenumber were used. In the selected range, only spectra correlated to the vibration peaks of functional groups from MOSO were selected such as 3010-2835 cm^{-1}, 2935-2830 cm^{-1}, 1800-710 cm^{-1}, and their combination. After the optimization procedure in terms of selection of wavenumbers regions, the types of multivariate calibration and FTIR spectral treatments, finally PLSR using normal spectra of the combined infrared region of 2935-2830 and 1800-710 cm^{-1} was selected for quantitative modelling. Using this condition, PLSR offered the best model for predicting the levels of Sy-O, having the highest R^2-calibration value (0.9855), R^2-validation value (0.9839), and lowest RMSEC value (1.67 %) and lowest RMSEP value (1.69 %). Fig. 4 revealed PLSR models either in calibration [A] or in validation [B] models which correlated the actual values of Sy-O in MOSO and FTIR predicted values. Previous study also reported the benefits on using PLSR for predicting adulterants in edible oils. For instance, the adulteration of pumpkin seed oils using refined rapeseed oil was successfully detected and predicted using FTIR spectroscopy and PLSR [42]. In addition, PLSR in combination with FTIR spectroscopy was successfully used to detect and quantify argemone oil adulteration in virgin coconut oil with outstanding R^2 value (0.999) [43]. Authentication of extra virgin olive oil adulteration from grapeseed oil, walnut oil, and soybean oil has also been successfully performed using FTIR spectroscopy in combination with PLSR with R^2 larger than 0.990 [44].

Discriminant analysis (DA) is further used for the classification between authentic MOSO and MOSO added with Sy-O as adulterant. DA is a supervised pattern recognition technique employed for the classification of authentic samples and those adulterated with others. Fig. 5 showed the Coomans plot calculated based on the Mahalanobis distance of MOSO adulterated with Sy-O using the absorbance values used in PLSR model (the combined wavenumbers regions of 2935-2830 and 1800-710 cm^{-1}). The *x-axis* shows the Mahalanobis distance of authentic MOSO to the adulterated MOSO, while the *y-axis* shows the Mahalanobis distance of the adulterated oil to the authentic MOSO. All data points are clustered according to its groups without any misclassified objects. This indicated that DA could classify the authentic MOSO and that adulterated with Sy-O with accurate results, even at low concentrations (1.25 % v/v).

This study showed the potential and advantage use of FTIR spectroscopy in combination with chemometrics to detect adulterant (Sy-O) in MOSO using the absorbance values from the FTIR spectra. The chemometrics of PLSR provided a good model with high accuracy and precision to detect and predict the levels of Sy-O added in MOSO. In addition, the DA analysis could clearly discriminate pure and adulterated MOSO with Sy-O. It indicated that FTIR spectroscopy and chemometrics are promising as a rapid and effective analytical method for authentication of MOSO.

4. Conclusions

In this study, the physico-chemical characterization and authentication analysis using FTIR spectroscopy and chemometrics of *Moringa oleifera* seed oil was performed. It was found that MOSO from different regions had a good physico-chemical properties in terms of acid values (0.32 ± 0.01 mg KOH/g MOSO), saponification values (182.50 ± 5.95 mg KOH/g MOSO), iodine values (78.30 ± 4.24 g I_2/100 g MOSO), and peroxide values (1.12 ± 0.02 meq O_2/kg MOSO). In addition, the determination of fatty acid composition of MOSO from various origins using GC-FID showed that oleic acid (C18:1) and palmitic acid (C16:0) were the dominant fatty acids found in MOSO accounted for 68.31–76.89 % and 6.17–8.27 %, respectively. On the other hand, the chemometrics of PLS-DA using variables of fatty acids successfully discriminated and classified MOSO into group 1 and group 2. On the other hand, the authentication of MOSO from soybean adulteration was performed using FTIR spectroscopy and chemometrics of partial least regression (PLSR). Using the combination of wavenumbers region of 2935-2830 and 1800-710 cm^{-1}, PLSR successfully predicted the levels of Sy-O added in MOSO with coefficient of determination (R^2) in calibration and validation models were of 0.9971 and 0.9961, respectively associated to the high model accuracy. In addition, the PLSR model had low error with root mean square error of calibration (RMSEC) and root mean square error of prediction (RMSEP) of 1.67 % and 1.93 %,

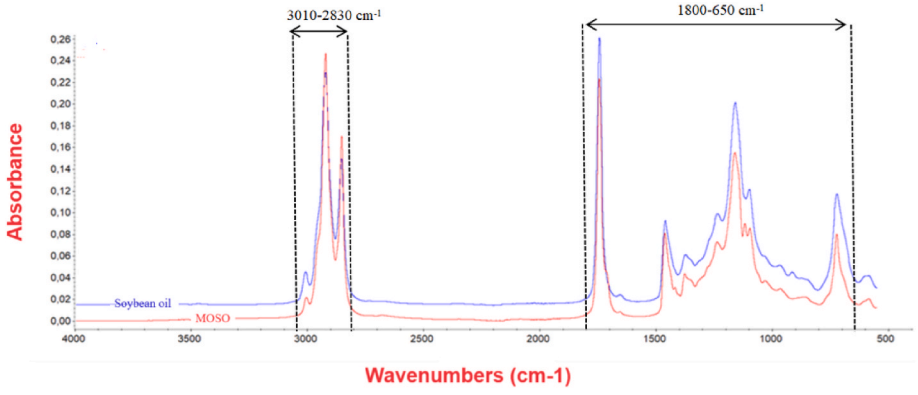

Fig. 3. Attenuated total reflectance-FTIR spectral regions where variations between *Moringa oleifera* seed oil (MOSO) and soybean oil (Sy-O) existed, namely at wavenumbers of 3010-2830 cm^{-1} and at 1800-650 cm^{-1}.

Table 2
The statistical performances of the partial least square calibration (PLSR) and principle component regression (PCR) for making the prediction models of soybean oil as adulterant in Moringa oleifera seed oil (MOSO) at different regions and FTIR spectral treatments.

Wave number (cm^{-1})	Multivariate calibration	FTIR spectra[a]	Factor (PC)	Equation		R^2		RMSEC (%)	RMSEP (%
				Calibration	Validation	Calibration	Validation		
3010–650	PLS	Normal	3	y = 0.9921x + 0.206	y = 0.9878x + 0.0371	0.9961	0.9957	1.93	2.04
		1st der.	2	y = 0.9916x + 0.2215	y = 0.9839x + 0.1959	0.9958	0.9951	2.00	2.18
		2nd der.	3	y = 0.9929x + 0.1877	y = 0.9838x + 0.2601	0.9964	0.9958	1.85	2.01
	PCR	Normal	10	y = 0.9925x + 0.1969	y = 0.9907x - 0.0588	0.9963	0.9960	1.88	1.98
		1st der.	10	y = 0.9929x + 0.1874	y = 0.988x + 0.038	0.9964	0.9956	1.84	2.05
		2nd der.	10	y = 0.993x + 0.1836	y = 0.9903x + 0.0877	0.9965	0.9956	1.82	2.06
3010–2835	PLS	Normal	3	y = 0.9775x + 0.5904	y = 0.9682x + 0.0831	0.9887	0.9859	3.27	3.73
		1st der.	3	y = 0.9909x + 0.2382	y = 0.985x + 0.1017	0.9955	0.9945	2.08	2.30
		2nd der.	3	y = 0.9918x + 0.2172	y = 0.9923x + 0.1736	0.9959	0.9959	1.98	1.96
	PCR	Normal	5	y = 0.992x + 0.2095	y = 0.9766x + 0.4768	0.9960	0.9961	1.95	1.96
		1st der.	5	y = 0.9929x + 0.1846	y = 0.9884x + 0.1866	0.9965	0.9963	1.83	1.88
		2nd der.	5	y = 0.9929x + 0.1846	y = 0.9884x + 0.1866	0.9964	0.9963	1.84	1.87
1800–710	PLS	Normal	4	y = 0.992x + 0.2102	y = 0.9846x - 0.2403	0.9960	0.9960	1.95	1.96
		1st der.	3	y = 0.9915x + 0.2226	y = 0.9873x + 0.2951	0.9957	0.9959	2.01	1.97
		2nd der.	2	y = 0.9909x + 0.2393	y = 0.9847x + 0.3231	0.9954	0.9953	2.08	2.13
	PCR	Normal	5	y = 0.9918x + 0.2158	y = 0.9895x + 0.0111	0.9959	0.9960	1.97	1.98
		1st der.	5	y = 0.9921x + 0.2077	y = 0.9853x + 0.2488	0.9960	0.9955	1.94	2.07
		2nd der.	5	y = 0.992x + 0.2094	y = 0.9816x + 0.3902	0.9960	0.9953	1.96	2.11
2935–2830 and 1800–710[b]	**PLS**	Normal	**5**	**y = 0.9941x + 0.154**	**y = 0.9989x + 0.0658**	**0.9971**	**0.9961**	**1.67**	**1.93**
		1st der.	3	y = 0.9925x + 0.1955	y = 0.9859x + 0.1876	0.9962	0.9957	1.89	2.02
		2nd der.	3	y = 0.9927x + 0.1902	y = 0.9858x + 0.2356	0.9964	0.9959	1.86	1.97
	PCR	Normal	10	y = 0.9948x + 0.1354	y = 1.0051x - 0.243	0.9974	0.9973	1.57	1.63
		1st der.	10	y = 0.9964x + 0.0958	y = 0.9979x - 0.0541	0.9982	0.9979	1.31	1.42
		2nd der.	10	y = 0.9955x + 0.1184	y = 0.9928x + 0.081	0.9977	0.9975	1.47	1.56

[a] 1st der. = 1st derivative; 2nd der. = 2nd derivative.
[b] **The condition selected for making the calibration and validation models was marked with bold.**

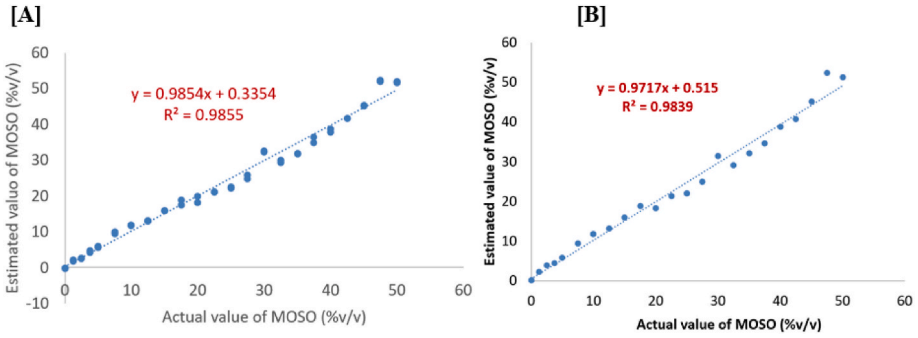

Fig. 4. Partial least squares regression (PLSR) models either in calibration [A] or in validation [B] models which correlated the actual values of soybean oil (Sy-O) in *Moringa oleifera* seed oil (MOSO) and FTIR predicted values.

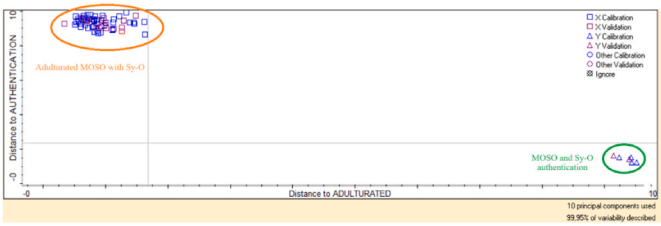

Fig. 5. Discriminant analysis of authentic *Moringa oleifera* seed oils (MOSO) and those adulterated with soybean oil (Sy-O).

respectively, indicating good precision models. It can be concluded that MOSO contained good and important physico-chemical properties including fatty acid compositions which are beneficial for its further applications in pharmaceutical, nutraceutical, and cosmetical products. In addition, the FTIR spectroscopy in combination with chemometrics is very promising to be used as a rapid and effective analytical technique for authentication of MOSO from oil adulterants. For the next, research using larger samples is required to warrant the reproducibility of the results. In the future, this research is important for the food industry to combat high quality of edible adulteration and to ensure the product authenticity. In addition, validating this technique for other high-value oils is important for quality control and authentication purposes.

CRediT authorship contribution statement

Irnawati: Writing – review & editing, Visualization, Resources, Project administration, Formal analysis, Writing – review & editing, Visualization, Resources, Project administration, Formal analysis. **Abdul Rohman:** Writing – review & editing, Writing – original draft, Supervision, Funding acquisition, Conceptualization. **Yamin:** Validation, Formal analysis, Data curation, Validation, Formal analysis, Data curation. **Nurrulhidayah Ahmad Fadzillah:** Supervision, Resources, Investigation. **Aida Azrina Azmi:** Writing – review & editing, Conceptualization. **Nurlatifah:** Formal analysis, Data curation, Formal analysis, Data curation. **Anjar Windarsih:** Writing – review & editing, Writing – original draft, Conceptualization. **Ratna Asmah Susidarti:** Writing – review & editing, Supervision, Conceptualization. **Ruslin:** Supervision, Conceptualization, Supervision, Conceptualization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgement

The authors thank the Directorate of Research Universitas Gadjah Mada for the financial support during this study through Post-Doctoral Program 2024 with a commitment letter of 4292/UN1.P1/PT.01.03/2024.

Data availability

Data will be made available on request.

References

[1] Z. Li, et al., Moringa oleifera Lam. leaf improves constipation of rats induced by low-fiber-diet: a proteomics study, J. Ethnopharmacol. 318 (2024) 116936, https://doi.org/10.1016/j.jep.2023.116936.
[2] W. Raja, K. Bera, B. Ray, Polysaccharides from Moringa oleifera Gum: structural elements, interaction with beta-blactoglobulin and antioxidative activity, RSC Adv. 6 (2016) 75699–75706, https://doi.org/10.1039/C6RA13279K.
[3] C. Chen, B. Zhang, Q. Huang, X. Fu, R. Hai, Microwave-assisted extraction of polysaccharides from Moringa oleifera lam. leaves: characterization and hypoglycemic activity, Ind. Crops Prod. 100 (2017) 1–11, https://doi.org/10.1016/j.indcrop.2017.01.042.
[4] H. Tian, et al., International journal of biological macromolecules Moringa oleifera polysaccharides regulates caecal microbiota and small intestinal metabolic pro fi le in c57bl/6 mice, Int. J. Biol. Macromol. 182 (2021) 595–611, https://doi.org/10.1016/j.ijbiomac.2021.03.144.
[5] M. Nadeem, M. Imran, Promising features of Moringa oleifera oil: recent updates and perspectives, Lipids Health Dis. 15 (2016) 1–8, https://doi.org/10.1186/s12944-016-0379-0.
[6] S. Lalas, J. Tsaknis, Extraction and identification of natural antioxidant from the seeds of the Moringa oleifera tree variety of Malawi, JAOCS, J. Am. Oil Chem. Soc. 79 (2002) 677–683, https://doi.org/10.1007/s11746-002-0542-2.
[7] P. Siddhuraju, K. Becker, Antioxidant properties of various solvent extracts of total phenolic constituents from three different agroclimatic origins of drumstick tree (Moringa oleifera Lam.) leaves, J. Agric. Food Chem. 51 (2003) 2144–2155, https://doi.org/10.1021/jf020444+.
[8] S.M. Abdulkarim, O.M. Lai, S.K.S. Muhammad, K. Long, H.M. Ghazali, Oleic acid enhancement of Moringa oleifera seed oil by enzymatic transesterification and fractionation, Int. Food Res. J. 14 (2007) 91–102.
[9] C. Wen, et al., Edible vegetable oils from oil crops: preparation, refining, authenticity identification and application, Process Biochem. 124 (2023) 168–179, https://doi.org/10.1016/j.procbio.2022.11.017.
[10] J. Fakhfakh, S. Ben-Youssef, Mu Naushad, N. Allouche, Different Extraction Methods, Physical Properties and Chemical Composition of Date Seed Oil, 2019, pp. 125–153, https://doi.org/10.1007/978-3-030-11345-2_7.
[11] J. Fakhfakh, S. Ben-Youssef, Mu Naushad, N. Allouche, Different Extraction Methods, Physical Properties and Chemical Composition of Date Seed Oil, 2019, pp. 125–153, https://doi.org/10.1007/978-3-030-11345-2_7.
[12] B. Ladjouze, A. Kribeche, M. Takka, L. Boulekbache-makhlouf, K. Madani, Optimization of ultrasonic assisted extraction of oil from Moringa oleifera shelled and unshelled seeds, South Afr. J. Bot. 163 (2023) 684–691, https://doi.org/10.1016/j.sajb.2023.11.004.
[13] C. Chen, B. Zhang, Q. Huang, X. Fu, R. Hai, Microwave-assisted extraction of polysaccharides from Moringa oleifera lam. leaves: characterization and hypoglycemic activity, Ind. Crops Prod. 100 (2017) 1–11, https://doi.org/10.1016/j.indcrop.2017.01.042.
[14] S. Zhao, D. Zhang, A parametric study of supercritical carbon dioxide extraction of oil from Moringa oleifera seeds using a response surface methodology, Separ. Purif. Technol. 113 (2013) 9–17, https://doi.org/10.1016/j.seppur.2013.03.041.
[15] A. Rohman, et al., Comprehensive review on application of FTIR spectroscopy coupled with chemometrics for authentication analysis of fats and oils in the food products, Molecules 25 (2020) 1–28.
[16] F.N. Dos Santos, et al., Immediate differentiation of unusual seed oils by easy ambient sonic-spray ionization mass spectrometry and chemometric analysis, Anal. Methods 8 (2016) 3681–3690, https://doi.org/10.1039/c5ay03061g.
[17] A. Rohman, A.R. Putri, Irnawati, A. Windarsih, K. Nisa, L.A. Lestari, The employment of analytical techniques and chemometrics for authentication of fish oils: a review, Food Control 124 (2021).
[18] N. Mialon, B. Roig, E. Capodanno, A. Cadiere, Untargeted metabolomic approaches in food authenticity: a review that showcases biomarkers, Food Chem. 398 (2023) 133856, https://doi.org/10.1016/j.foodchem.2022.133856.
[19] J.M.N. Marikkar, N. Kamil, A.R. Raihana, Differential scanning calorimetric analysis of virgin coconut oil, palm olein, and their adulterated blends, Cordulia 35 (2019) 9, https://doi.org/10.37833/cord.v35i01.10.
[20] Z. Haddi, et al., Electronic nose and tongue combination for improved classification of moroccan virgin olive oil profiles, Food Res. Int. 54 (2013) 1488–1498, https://doi.org/10.1016/j.foodres.2013.09.036.
[21] A. Rohman, Y.B.C. Man, Application of Fourier transform infrared spectroscopy for authentication of functional food oils, Appl. Spectrosc. Rev. 47 (2012) 1–13, https://doi.org/10.1080/05704928.2011.619020.
[22] A. Rohman, Y.B. Che Man, Authentication of extra virgin olive oil from sesame oil using FTIR spectroscopy and gas chromatography, Int. J. Food Prop. 15 (2012), https://doi.org/10.1080/10942912.2010.521607.
[23] A. Rohman, et al., Fourier transform infrared spectroscopy combined with multivariate calibrations for the authentication of avocado oil, Int. J. Food Prop. 19 (2016) 680–687, https://doi.org/10.1080/10942912.2015.1039029.
[24] A. Rohman, Y.B.C. Man, S. Riyanto, Authentication analysis of red fruit (Pandanus conoideus lam) oil using FTIR spectroscopy in combination with chemometrics, Phytochem. Anal. 22 (2011) 462–467, https://doi.org/10.1002/pca.1304.
[25] C. Huynh Mai, H. Cang Mai, T. Thanh Truc Le, T. Yen Nhi Bui, Maceration extraction of oil from tamanu (Calophyllum inophyllum l.) seeds: effect of process parameters and oil characterisations, Int. J. Eng. Res. Afr. 10 (2020) 31–39, https://doi.org/10.9790/9622-1006033139.
[26] R.B. Pebriana, A. Rohman, E. Lukitaningsih, Sudjadi, Development of FTIR spectroscopy in combination with chemometrics for analysis of rat meat in beef sausage employing three lipid extraction systems, Int. J. Food Prop. 20 (2017) 1–11, https://doi.org/10.1080/10942912.2017.1361969.
[27] A. Rohman, Y.B.C. Man, Palm oil analysis in adulterated sesame oil using chromatography and ftir spectroscopy, Eur. J. Lipid Sci. Technol. 113 (2011) 522–527, https://doi.org/10.1002/ejlt.201000369.
[28] A. Rohman, Y.B. Che Man, F.M. Yusof, The use of FTIR spectroscopy and chemometrics for rapid authentication of extra virgin olive oil, JAOCS, J. Am. Oil Chem. Soc. 91 (2014), https://doi.org/10.1007/s11746-013-2370-5.
[29] Y.B. Che Man, A. Rohman, T.S.T. Mansor, Differentiation of lard from other edible fats and oils by means of Fourier transform infrared spectroscopy and

chemometrics, JAOCS, J. Am. Oil Chem. Soc. 88 (2011) 187–192, https://doi.org/10.1007/s11746-010-1659-x.
[30] M.M. Özcan, Moringa Spp: composition and bioactive properties, South Afr. J. Bot. 129 (2020) 25–31, https://doi.org/10.1016/j.sajb.2018.11.017.
[31] A.A. Aly, R.W. Maraei, H.G.M. Ali, Fatty acids profile and chemical composition of Egyptian Moringa oleifera seed oils, JAOCS, J. Am. Oil Chem. Soc. 93 (2016) 397–404, https://doi.org/10.1007/s11746-015-2781-6.
[32] B.S. Ogunsina, T.N. Indira, A.S. Bhatnagar, C. Radha, S. Debnath, A.G. Gopala Krishna, Quality characteristics and stability of Moringa oleifera seed oil of Indian origin, J. Food Sci. Technol. 51 (2014) 503–510, https://doi.org/10.1007/s13197-011-0519-5.
[33] K. Gharsallah, L. Rezig, K. Msaada, A. Chalh, T. Soltani, Chemical composition and profile characterization of Moringa oleifera seed oil, South Afr. J. Bot. 137 (2023) 475–482, https://doi.org/10.1016/J.SAJB.2020.11.014.
[34] M. Haile, H.T. Duguma, G. Chameno, C.G. Kuyu, Effects of location and extraction solvent on physico chemical properties of Moringa stenopetala seed oil, Heliyon 5 (2019) e02781, https://doi.org/10.1016/J.HELIYON.2019.E02781.
[35] B. Worley, S. Halouska, R. Powers, Utilities for quantifying separation in PCA/PLS-DA scores plots, Anal. Biochem. 433 (2013) 102–104, https://doi.org/10.1016/j.ab.2012.10.011.
[36] A.M. Jiménez-Carvelo, S. Martín-Torres, F. Ortega-Gavilán, J. Camacho, PLS-DA vs Sparse PLS-DA in food traceability. a case study: authentication of avocado samples, Talanta 224 (2021) 121904, https://doi.org/10.1016/J.TALANTA.2020.121904.
[37] B. Worley, R. Powers, Multivariate analysis in metabolomics, Curr Metabolomics 1 (2013) 92–107, https://doi.org/10.2174/2213235x11301010092.
[38] L. Yuan, et al., A comparative study on classification of edible vegetable oils by infrared, near infrared and fluorescence spectroscopy combined with chemometrics, Spectrochim. Acta Mol. Biomol. Spectrosc. 288 (2023) 122120, https://doi.org/10.1016/J.SAA.2022.122120.
[39] E. Sufriadi, R. Idroes, H. Meilina, A.A. Munawar, N. Lelifajri, G. Indrayanto, Partial least squares-discriminant analysis classification for patchouli oil adulteration detection by Fourier transform infrared spectroscopy in combination with chemometrics, ACS Omega 8 (2023) 12348–12361, https://doi.org/10.1021/ACSOMEGA.3C00080/ASSET/IMAGES/LARGE/AO3C00080_0008.JPE.
[40] Z.A. Syahariza, Y.B. Che Man, J. Selamat, J. Bakar, Detection of lard adulteration in cake formulation by fourier transform infrared (FTIR) spectroscopy, Food Chem. 92 (2005) 365–371, https://doi.org/10.1016/j.foodchem.2004.10.039.
[41] J. Moros, S. Garrigues, M. de la Guardia, Vibrational spectroscopy provides a green tool for multi-component analysis, TrAC, Trends Anal. Chem. 29 (2010) 578–591, https://doi.org/10.1016/j.trac.2009.12.012.
[42] C. Lörchner, C. Fauhl-Hassek, M.A. Glomb, V. Baeten, J.A. Fernández Pierna, S. Esslinger, Comparison of spectroscopic techniques using the adulteration of pumpkin seed oil as example, Food Anal. Methods 17 (2024) 332, https://doi.org/10.1007/S12161-023-02568-4/TABLES/2, 247.
[43] S. Kumari, D. Kumar Singh, Swift and precise detection of argemone oil adulteration in virgin coconut oil by implementing ATR-FTIR spectroscopy integrated with multivariate chemometrics and regression modelling, Vib. Spectrosc. 126 (2023) 103525, https://doi.org/10.1016/j.vibspec.2023.103525.
[44] A. Rohman, Y. bin Che Man, A. Ismail, P. Hashim, FTIR spectroscopy coupled with chemometrics of multivariate calibration and discriminant analysis for authentication of extra virgin olive oil, Int. J. Food Prop. 20 (2017) S1173–S1181, https://doi.org/10.1080/10942912.2017.1336718.