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Rapid Authentication of Bandeng (*Chanos chanos*) Oil Nanoemulsion Using Fourier Transform Infrared (FTIR) Spectroscopy Combined with Chemometrics

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Abstract

A high level of polyunsaturated fatty acid (PUFA) in bandeng oil nanoemulsion (BON) makes it risky to be adulterated using low-quality oils such as palm oil (PO). Authentication of BON is essential to guarantee product quality and safety. Adulterated nanoemulsion is particularly challenging to identify because the surfactant matrix and aqueous phase mask the characteristic odor, color, and specific chemical markers detectable in bulk oils. This research aims to perform the authentication of BON using FTIR spectroscopy combined with chemometrics. Adulteration models were built using palm oil as an adulterant, bandeng oil as a pure component, and nanoemulsion matrix. All samples were analyzed using ATR-FTIR spectroscopy at 4000–650 cm^{-1} wavenumbers. Chemometrics technique, such as principal component analysis (PCA), partial least squares regression (PLSR), and principal component regression (PCR), was performed to separate and quantify BON from adulterant. PCA successfully separated BON from palm oil (PO) as an adulterant. Therefore, PLSR using normal spectra at wavenumbers 1500–650 cm^{-1} had the best value based on highest R^2_{cal} value 0.9503; R^2_{pred} value 0.8761; lowest RMSEC 0.145; RMSEP 0.245. It can be concluded that FTIR spectroscopy combined with chemometrics was claimed as rapid, accurate, and suitable for authenticating BON from PO as an adulterant in nanoemulsion form.

Keywords: Fish oil nanoemulsion, Fingerprint, Partial least squares regression, Principal component analysis, Principal component regression



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Introduction

Fish oils are known as sources of polyunsaturated fatty acids (PUFA) and essential omega-3 unsaturated fatty acids such as eicosapentaenoic acid (EPA) and docosahexaenoic acid (DHA). Fish oils come mainly from oily fishes, such as cod, salmon, sardine, anchovy, and mackerel (Nieva-Echevarría, Goicoechea, & Guill'en, 2017; Chandrasekar, Belur, & Regupathi, 2018). Omega-3 fatty acid consumption has several beneficial effects on human health, such as antioxidant activity (Ikhsan, Syifa, Mustafidah, & Rohman, 2021) being recognized as effective against cardiovascular and inflammatory diseases, among others (Nichols, McManus, Krail, Sinclair, & Miller, 2014).

Recently, bandeng oil has been the focus of growing interest due to its nutritional advantages. Bandeng had a good quantity of protein, amino acids, vitamins, and polyunsaturated fatty acids. It contains rich levels of unsaturated fatty acids (50.74%), with monounsaturated fatty acids (MUFA) and polyunsaturated fatty acids (PUFA) constituting 34.47 and 16.27%, respectively (Murthy *et al.*, 2016). Therefore, oil extracted from bandeng has the potential to be developed as a source of fish oil.

Bandeng oil has large-scale market potential. First, it can be the source of vitamin A and D and the long-chain n-3 fatty acids. Fish-oil products based on natural fish oil or their derivatives are frequently introduced to the market as a functional food (emulsion) or medicines, because consumption of seafood directly may be attributed to taste, price, contamination concerns such as heavy metals, and availability (Kennedy, Luo, & Ausman, 2012). Nanoemulsion-based delivery systems offer many potential benefits for incorporating omega-3 oils into foods and beverages. Fish oil nanoemulsion has been introduced to enrich foodstuffs, including meat, bakery, and dairy products such as yogurt (Zhong, Yang, Cao, Liu, & Qin, 2018; Jamshidi, Cao, Xiao, Simal-Gandara, 2020). The nanoemulsion

method can effectively improve the oxidative stability of fish oil and mask unpleasant fishy flavour in fortified products.

Authentication of bandeng oil nanoemulsion (BON) is essential to prevent adulteration, ensure quality, nutritional value, and product safety for consumers. Driven by economic, unethical fats and oils, producers may intentionally or unintentionally mislabel and adulterate high-quality fish oils (Rohman, Putri, Irnawati Windarsih, Nisa, & Lestari, 2021). Adulteration involves the addition of cheaper oils. The potential adulterants of fish oil nanoemulsion are plant oils or vegetable oils. Fish oil is mainly adulterated using palm oil (PO) because of its physicochemical property similarities and lower prices (Putri, Rohman, & Riyanto, 2019).

Due to the increasing demand for fish oil nanoemulsions, it is essential to have a fast and accurate method to verify identification and detection of potential adulterants. Analytical methods that can be employed for authentication are gas chromatography-mass spectrometry (GC-MS) (Gul, Nasrullah, Nissar, Saifi, & Abdin, 2018), nuclear magnetic resonance (NMR) (Amargianitaki & Spyros, 2017), ultraperformance liquid chromatography (UPLC) (Setyaningsih, Saputro, Carrera, Palma, & García-Barroso, 2019), and Fourier transform infrared (FTIR) spectroscopy (Putri *et al.*, 2019; Ikhsan *et al.*, 2021b). While GC-MS, NMR, and UPLC offer high specificity, they are often associated with higher costs, longer analysis times, and more complex sample preparation, making them less suitable for rapid, high-throughput screening. FTIR spectroscopy, in contrast, provides a fast, solvent-free, and cost-effective alternative suitable for routine authentication.

FTIR spectroscopy is the most commonly used technique to determine authentication analysis, especially in fats and oils. It is also considered green analytical chemistry because it requires less solvent (Choiri, Sulaiman, & Rohman, 2020; Ikhsan *et al.*, 2021b). FTIR spectroscopy combined with multivariate analysis has been applied for authentication of

virgin olive oil (Tay, Singh, Krishnan, & Gore, 2002), virgin coconut oil (Manaf, Che Man, Hamid, Ismail, & Abidin, 2007), and snakehead fish oil (Syifa, Irnawati, Riyanta, & Rohman, 2020). However, a literature search suggests that there is no information available related to the use of FTIR spectroscopy in BON, especially related to authentication.

The objective of this study is to authenticate BON that has been adulterated with palm oil using FTIR spectroscopy combined with chemometrics. Further analysis was conducted to distinguish BON as a pure product, and palm oil nanoemulsion (PON) as well as mixture oil nanoemulsion (MON) as fake products based on their FTIR spectra using the principal component analysis (PCA) method. However, partial least squares regression (PLSR) and principal component regression (PCR) calibration were intended for quantitative analysis adulteration models.

Materials and Methods

Bandeng was obtained from a local fish breeder in Pati, Central Java, Indonesia. Fish oil extraction was conducted in Sekolah Pasca Sarjana, Universitas Gadjah Mada, Yogyakarta, Indonesia. Meanwhile, the palm oil and other nanoemulsion components were purchased from Brataco (Yogyakarta, Indonesia).

Preparation of Adulteration Model's

Fish oil adulteration models were prepared by mixture bandeng oil and palm oil at varying concentrations ranging from 0% to 100% (v/v), as randomly generated using Excel software (Microsoft Inc, USA) (Mustafidah, Irnawati, Lukitaningsih, & Rohman, 2021). A total of 25 mixture samples (MON) were prepared with different bandeng-to-palm oil ratios, along with three replicates each of pure bandeng oil nanoemulsion (BON) and pure palm oil nanoemulsion (PON), resulting in 31 samples in total (Table 1).

Nanoemulsions were formulated according to a low-energy emulsification method (Chong *et al.*, 2018). Each oil mixture was combined

with 1500 μL Tween 80, 500 μL Span 80, and 16,000 μL distilled water, then premixed using a magnetic stirrer hotplate (IKA C MAG HS 7) at 800 rpm and 60 $^{\circ}\text{C}$ for 10 min. Subsequent homogenization was performed at 15,000 rpm for 5 min with a high-speed disperser (Ultra-Turrax T25, IKA). The resulting nanoemulsions were stored at 4 $^{\circ}\text{C}$ until further analysis. All samples were prepared in three independent batches over two separate days to account for preparation variability.

FTIR Spectroscopy Analysis

An FTIR spectrophotometer (Thermo Scientific Nicolet iS10, Madison, WI) was used to analyze all nanoemulsion samples based on Putri *et al.* (2019) research. Various wavenumber between 4000 – 650 cm^{-1} was used for measurement using 16 cm^{-1} resolution and each spectrum was the average of 32 scans to ensure a high signal-to-noise ratio (Rohman *et al.*, 2020). Horizontal Attenuated Total Reflectance (HATR) composed ZnSe crystal was used for sampling accessory. Before analyzing each sample, a correction was performed by scanning a background spectrum of room air in the same condition. The sampling accessory was cleaned using n-hexane and acetone after FTIR spectrophotometer analysis was conducted.

Data Matrix Construction and Spectral Processing

The spectral data were organized into a matrix of dimensions 31×1680 , where rows represented individual samples (25 MON, 3 PON, 3 BON) and columns corresponded to the 1680 absorbance values acquired across the wavenumber range of 4000–650 cm^{-1} . Prior to chemometric analysis, the raw spectra were preprocessed using baseline correction (linear baseline fit between 1800 cm^{-1} and 800 cm^{-1}) followed by vector normalization (standard normal variate, SNV) to minimize scattering effects and enhance spectral comparability. For derivative spectra, Savitzky-Golay filtering with a 9-point window and second-order polynomial was

used to compute first and second derivatives. Wavenumber selection was performed by evaluating several spectral sub-regions based on their chemical relevance and signal-to-noise ratio. The range 1500–650 cm^{-1} was identified as optimal for

modeling, as it contains characteristic bands of lipid functional groups (e.g., C=O stretching, C–H bending) and showed the highest discriminative power in preliminary PCA (Crouse, Rousseau, & Grover, 2024).

Table 1- Composition of nanoemulsion samples used in adulteration models: milkfish oil and palm oil mixtures

Sample Codes	Milkfish oil (μL)	Palm oil (μL)	Tween80 (μL)	Span80 (μL)	Distilled water (μL)
MON1	590	1410	1500	500	16000
MON2	280	1720	1500	500	16000
MON3	960	1040	1500	500	16000
MON4	140	1860	1500	500	16000
MON5	290	1710	1500	500	16000
MON6	850	1150	1500	500	16000
MON7	660	1340	1500	500	16000
MON8	1590	410	1500	500	16000
MON9	1470	530	1500	500	16000
MON10	380	1620	1500	500	16000
MON11	640	1360	1500	500	16000
MON12	480	1520	1500	500	16000
MON13	630	1370	1500	500	16000
MON14	1310	690	1500	500	16000
MON15	560	1440	1500	500	16000
MON16	840	1160	1500	500	16000
MON17	920	1080	1500	500	16000
MON18	860	1140	1500	500	16000
MON19	430	1570	1500	500	16000
MON20	1260	740	1500	500	16000
MON21	1700	300	1500	500	16000
MON22	530	1470	1500	500	16000
MON23	1020	980	1500	500	16000
MON24	270	1730	1500	500	16000
MON25	280	1720	1500	500	16000
PON1	0	2000	1500	500	16000
PON2	0	2000	1500	500	16000
PON3	0	2000	1500	500	16000
BON1	2000	0	1500	500	16000
BON2	2000	0	1500	500	16000
BON3	2000	0	1500	500	16000

MON: Mixture oil nanoemulsion, PON: Palm oil nanoemulsion, BON: Bandeng oil nanoemulsion

Preparation of Calibration and Validation Samples

The samples for validation were prepared using the same spanned samples concentration as in samples for calibration. The validation was performed using the leave one out technique. The performance of the calibration models was evaluated using the following statistical parameters: The optimal number of PLSR and PCR was selected based on the minimum RMSECV (*Root mean square error*

of cross-validation). The model with the highest Coefficient of determination for calibration (R^2_{cal}) and prediction (R^2_{pred}), together with the lowest RMSEC (*Root mean square error of calibration*) and RMSEP (*Root mean square error of prediction*) was chosen for the authentication of bandeng oil nanoemulsion.

Chemometrics analysis

Principal component analysis (PCA) was performed using Minitab 19 (Minitab Inc.,

USA). Quantification partial least squares regression (PLSR) and principal component regression (PCR) was used for quantitative analysis using TQ Analyst™ (Thermo Fisher Scientific Inc., USA) (Miller & Miller, 2018). For PLSR and PCR, the number of latent variables (LVs) was selected based on the minimum RMSEC.

Results and Discussion

Generally, animal fats and oils can be differed based on the composition of fatty acids each fat and oils. The carbon chain length and unsaturation degree of different fatty acids can be detected using various analysis instruments such as high-performance liquid chromatography (HPLC), gas chromatography (GC), and Fourier transforms infrared (FTIR) spectroscopy (Fahy *et al.*, 2005). Therefore, using FTIR spectroscopy, adulteration practice can be detected using fingerprint FTIR spectra of each oil. FTIR spectroscopy was claimed rapid and effective in authenticating fish oil adulteration from

adulterants or different fish oils. However, in nanoemulsion form, various matrices from nanoemulsion surfactants and other components may affect the authentication method (Hertiani *et al.*, 2019; Kresnawati, Shantiningsih, & Martien, 2020).

The initial FTIR scanning was performed across the broad spectral range of 4000–650 cm^{-1} to capture the complete fingerprint region. However, to optimize the model for discrimination and quantification, a systematic wavenumber selection was conducted by comparing several spectral sub-regions: (1) the full range (4000–650 cm^{-1}), (2) the high-frequency region (3100–2800 cm^{-1}) associated with C–H stretching vibrations reflecting fatty acid chain length and unsaturation, (3) the fingerprint region (1800–650 cm^{-1}), and (4) a narrower fingerprint sub-region (1500–650 cm^{-1}). For each region, a PLSR model was built using normal spectra and evaluated by leave-one-out cross-validation (LOOCV) and independent external validation. The statistical results are summarized in Table 2.

Table 2- Performance of PLSR models built on different spectral regions (normal spectra).

Spectral region (cm^{-1})	LV	R ² cal	RMSEC	R ² pred	RMSEP
4000–650	7	0.892	0.210	0.801	0.312
3100–2800	4	0.745	0.335	0.689	0.421
1800–650	6	0.935	0.158	0.865	0.268
1500–650	5	0.9503	0.145	0.8761	0.245

LV: number of latent variables selected based on minimum RMSEC

The region 1500–650 cm^{-1} yielded the highest R²cal (0.9503) and R²pred (0.8761), along with the lowest RMSEC (0.145) and RMSEP (0.245). Although the region 2800–3100 cm^{-1} contains information about fatty acid chain length and unsaturation, it showed substantial spectral overlap between bandeng oil and palm oil in the nanoemulsion matrix. Moreover, a broad band around 3000–3500 cm^{-1} , due to O–H stretching from water

present in the nanoemulsion, introduced baseline variability that reduced discriminatory power. In contrast, the 1500–650 cm^{-1} region contains key functional group vibrations such as C=O stretching (~1745 cm^{-1}), C–H bending (~1465 cm^{-1}), and C–O stretching (~1160 cm^{-1}), which are more sensitive to differences in triglyceride composition.

Subsequently, within the selected region (1500–650 cm^{-1}), different spectral

preprocessing techniques were compared: normal spectra, first derivative, and second

derivative. The results for both PLSR and PCR are presented in Table 3.

Table 3- The optimization of multivariate calibration (PLSR and PCR) at 1500–650 cm⁻¹ wavenumber regions

	Wavelength (cm ⁻¹)	Spectra	RMSEC	R ² _{cal}	RMSEP	R ² _{pred}
		<i>Normal</i>	<i>0.145</i>	<i>0.9503</i>	<i>0.245</i>	<i>0.8761</i>
PLSR	1500-650	1 st derivative	0.256	0.8354	0.339	0.7120
		2 nd derivative	0.368	0.6144	0.400	0.5987
PCR	1500-650	Normal	0.276	0.8068	0.300	0.8109
		1 st derivative	0.335	0.6966	0.353	0.6747
		2 nd derivative	0.330	0.7061	0.370	0.6417

*The selection condition was marked with italicized bold

For the optimal PLSR model (1500–650 cm⁻¹, normal spectra), the calibration slope was 0.948 and the intercept was 0.025. The response variable (adulteration level) was expressed as the mass fraction of palm oil in the total oil phase, ranging from 0 to 1 (0–100%). Therefore, the RMSEC of 0.145 and RMSEP of 0.245 correspond to mean prediction errors of approximately 14.5% and 24.5% of the full adulteration range, respectively.

The lowest adulteration level tested was 10% palm oil (MON samples with 90% bandeng oil). The PLSR model showed acceptable prediction accuracy at this level (prediction error ~12%). The limit of detection (LOD) and limit of quantification (LOQ) were estimated as $3.3 \times \text{RMSEC} / \text{slope}$ and $10 \times \text{RMSEC} / \text{slope}$, yielding approximate values of 5% and 15% palm oil, respectively. This sensitivity is adequate for detecting economically motivated adulteration, which typically occurs at higher levels.

Partial least squares regression (PLSR) and principal component regression (PCR) can be observed in Table 3. In PLSR and PCR, linearity and error occurred was used to analyze the relationship between absorbance and concentration of each component. Statistical parameters, namely coefficient of determination for calibration (R²_{cal}), coefficient of determination for prediction (R²_{pred}), root mean square error of calibration

(RMSEC), as well as root mean square error of prediction (RMSEP) in normal spectra, 1st derivative spectra, and 2nd derivative spectra, were evaluated. RMSEC and R²_{cal} were used to evaluate calibration models; however, RMSEP and R²_{pred} were used to evaluate real cases and compared to the reference value obtained. For both PLSR and PCR, normal spectra provided the best performance. Therefore, the normal spectra in the 1500–650 cm⁻¹ region were used for the final quantitative adulteration models.

The method of choice for the authentication models was based on the highest values of coefficient of determination for calibration (R²_{cal}) and coefficient of determination for prediction (R²_{pred}), followed by the lowest values of root mean square error of calibration (RMSEC) and root mean square error of prediction (RMSEP). The normal spectra of FTIR spectra at wavenumbers of 1500 - 650 cm⁻¹ were the highest R²_{cal} values (0.9503); R²_{pred} (0.8761); followed by the lowest RMSEC (0.145), and the lowest RMSEP (0.245) using PLSR. Moreover, using PCR as the selection method resulted R²_{cal}; R²_{pred}; RMSEC; and RMSEP value was 0.8068; 0.8109; 0.276; and 0.300 respectively

The authentication method was performed using 4000 - 650 cm⁻¹ because fingerprint spectra can be observed in this area (Rohman *et al.*, 2020). The FTIR spectra of bandeng oil nanoemulsion (BON), palm oil nanoemulsion

(PON), and mixture oil nanoemulsion (MON) can be observed in Fig. 1. Moreover, in Fig. 1,

the various peaks corresponding to specific functional groups can be observed.

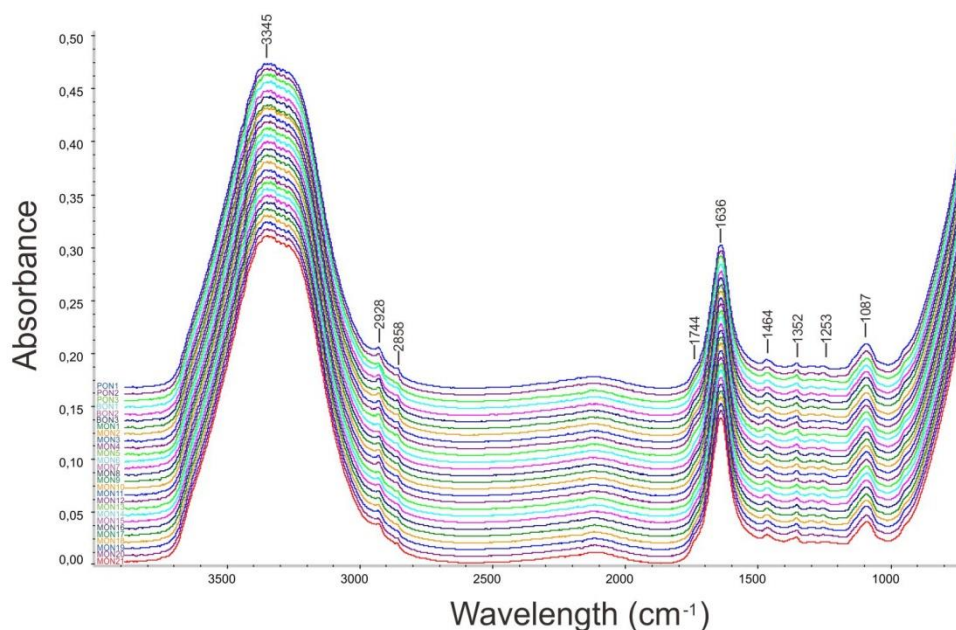


Fig. 1. The FTIR spectra of BON, PON, and MON at 4000 – 650 cm^{-1} wavenumber regions

Each peak and its functional group were compiled and observed in Table 4. A wide peak in every sample at 3000– 3500 cm^{-1} corresponds to water presence in nanoemulsion form. After wavenumber

optimization, the highest $R^2_{\text{cal}} - R^2_{\text{pred}}$ value and lowest RMSEP– RMSEC was obtained at 1500-650 cm^{-1} compared other wavenumber regions. Hence, this area can be used for quantitative analysis from adulteration models.

Table 4- Functional groups responsible in FTIR spectra between BON, PON, and MON at 4000 – 650 cm^{-1} wavenumber regions

Wavenumber (cm^{-1})	Functional Group
3345	-OH Stretch
2928	-CH ₂ stretch (asymmetric)
2858	-CH ₂ stretch (symmetric)
1744	-C=O ester stretch
1636	=C-H stretch (cis)
1464	-CH ₂ bending
1352	-CH ₃ bending
1253	-C-O ester stretch
1087	=C-H stretch (cis)

Principal component analysis (PCA) was used to discriminate each component from adulteration models at 4000– 650 cm^{-1} wavenumbers. PCA is an unsupervised pattern recognition that builds a discrimination model based on the similarity of the new variables (principal component) derived from wavenumber intensity as old variables (Miller

& Miller, 2018). Discrimination of the authentication model can be observed in Fig. 2. The bandeng oil nanoemulsion (BON), which was labelled as a pure product, was grouped in specific regions. However, palm fish oil nanoemulsion (PON), labeled as adulterated nanoemulsion, was grouped in other specific regions and located distant from

the BON group. It is caused by the difference of FTIR spectra between these two oils, in

which BON comes from animals and PON from plants.

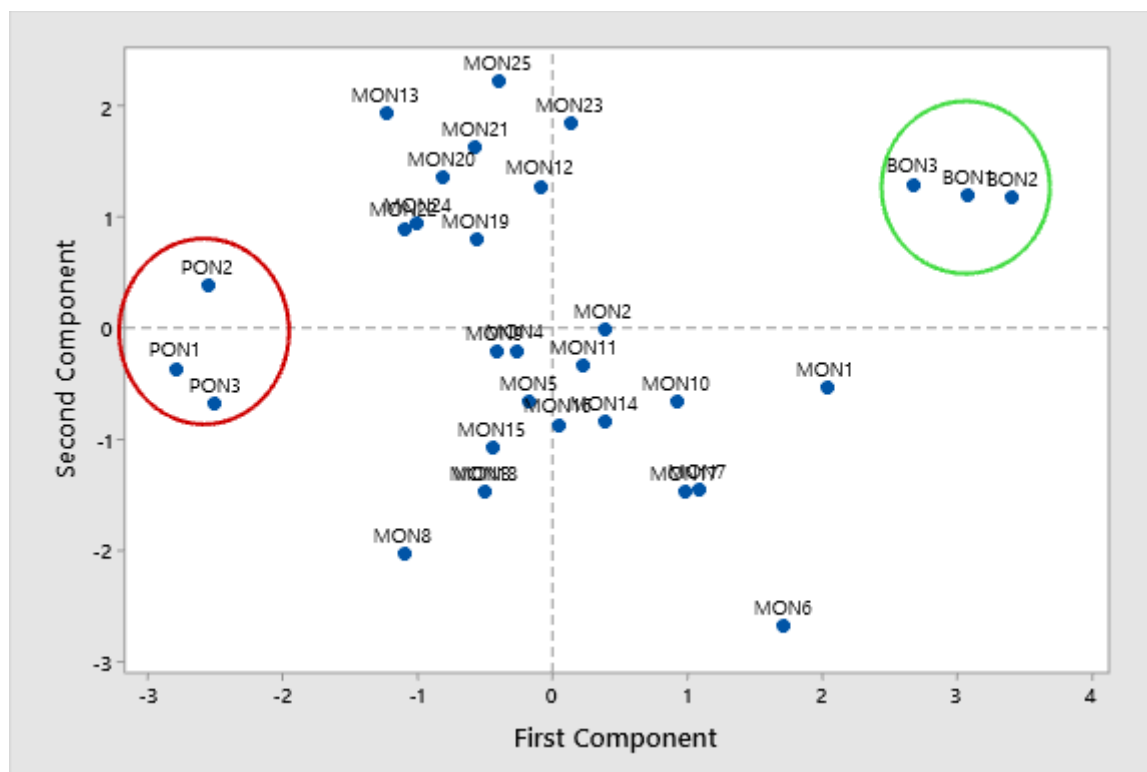


Fig. 2. The score plot between BON (green circle), PON (red circle), and MON

Based on the results, PCA has successfully discriminated BON from adulterant in the distant area between adulterants. The quantitative analysis using PLSR also yielded good analysis results, providing high accuracy and low errors method for the authentication of BON from PON as an adulterant in nanoemulsion form.

Conclusion

A combination of Fourier transform infrared (FTIR) spectroscopy with principal component analysis (PCA) and partial least squares regression (PLSR) was used for rapid authentication of BON. PCA discriminated and grouped BON from palm oil as an adulterant. The simultaneous analysis method was based on variable absorbances values of the normal spectra at 1500–650 cm^{-1} based on the highest accuracy and lowest errors. This

method was claimed rapid and effective to authenticate BON from PON as an adulterant.

Conflict of Interest

The authors declare no conflict of interest.

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Author Contributions

Masrukan: Conceptualization, Funding acquisition, Data curation, Formal analysis, Investigation, Methodology, Project administration, Resources, Supervision, Writing– original draft, Writing– review and editing. **Fitra Tunnisa:** Conceptualization,

Data curation, Formal analysis, Investigation, Software, Validation, Writing– original draft, Writing– review and editing. **Arif Nur Ikhsan:** Conceptualization, Investigation, Software, Validation, Visualization, Writing– original draft, Writing– review and editing.

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احراز هویت سریع نانوامولسیون روغن باندنگ (*Chanos chanos*) با استفاده از طیفسنجی مادون قرمز
تبدیل فوریه (FTIR) همراه با شیمیسنجی

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چکیده

سطح بالای اسید چرب چند غیراشباع (PUFA) در نانوامولسیون روغن باندنگ (BON)، تقلب در آن را با استفاده از روغن‌های بی کیفیت مانند روغن پالم (PO) خطرناک می‌کند. احراز هویت BON برای تضمین کیفیت و ایمنی محصول ضروری است. شناسایی نانوامولسیون تقلبی به‌ویژه چالش برانگیز است زیرا ماتریس سورفکتانت و فاز آبی، بو، رنگ و نشانگرهای شیمیایی خاص قابل تشخیص در روغن‌های قله را می‌پوشانند. هدف از این تحقیق، احراز هویت BON با استفاده از طیفسنجی FTIR همراه با شیمیسنجی است. مدل‌های تقلب با استفاده از روغن پالم به‌عنوان یک ماده تقلبی، روغن باندنگ به‌عنوان یک جزء خالص و ماتریس نانوامولسیون ساخته شدند. همه نمونه‌ها با استفاده از طیفسنجی ATR-FTIR در طول موج‌های ۴۰۰۰ تا ۶۵۰ (cm⁻¹) تجزیه و تحلیل شدند. تکنیک‌های شیمیسنجی، مانند تجزیه و تحلیل مؤلفه‌های اصلی (PCA)، رگرسیون حداقل مربعات جزئی (PLSR) و رگرسیون مؤلفه‌های اصلی (PCR)، برای جداسازی و تعیین کمیت BON از ماده تقلبی انجام شد. PCA با موفقیت BON را از روغن پالم (PO) به‌عنوان یک ماده تقلبی جدا کرد. بنابراین، PLSR با استفاده از طیف‌های نرمال در طول موج‌های ۱۵۰۰ تا ۶۵۰ (cm⁻¹)، بهترین مقدار R²cal برابر با ۰/۹۵۰۳، مقدار R²pred برابر با ۰/۸۷۶۱، کمترین RMSEC برابر با ۰/۱۴۵ و RMSEP برابر با ۰/۲۴۵ داشت. می‌توان نتیجه گرفت که طیفسنجی FTIR همراه با روش‌های شیمیسنجی، روشی سریع، دقیق و مناسب برای تشخیص BON از PO به‌عنوان یک ماده‌ی تقلبی در شکل نانوامولسیون است.

واژه‌های کلیدی: اثر انگشت، تحلیل مؤلفه‌های اصلی، رگرسیون حداقل مربعات جزئی، رگرسیون مؤلفه‌های اصلی، نانوامولسیون روغن ماهی

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