

Analysis of Virgin Coconut Oil (VCO) Purity Using UV-Vis Spectrophotometry Combined with PCA and HCA Chemometrics

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Abstract

VCO is a vegetable oil with many health and cosmetic benefits, but it is relatively more expensive than other vegetable oils, making it vulnerable to adulteration. UV-Vis spectrophotometry, combined with chemometric techniques, was used to distinguish VCO from other oils. Soybean oil (SO) and sunflower oil (SFO) are the main adulterants of VCO. This study aimed to evaluate the ability of UV-Vis spectrophotometry combined with chemometrics to differentiate VCO from SO and SFO. Samples were measured for absorbance at wavelengths from 200 to 400 nm. The UV-Vis spectral data were further analyzed using chemometric methods, PCA, and HCA, to classify the samples. The PCA model successfully differentiated VCO, SO, and SFO in RStudio 4.4.2, with variance explained by PC1 (81.3%) and PC2 (17.1%). VCO samples are clearly separated from other samples, while SO and SFO appear close to each other due to their similar physicochemical properties. Mixed oil samples were grouped by composition. HCA analysis also showed a grouping pattern consistent with PCA results. Therefore, UV-Vis spectrophotometry, combined with chemometric techniques, can effectively distinguish VCO from SO and SFO.

Keywords: chemometrics, UV-Vis spectrophotometry, virgin coconut oil

Analisis Kemurnian Minyak Kelapa Murni Menggunakan Spektrofotometri UV-Vis Kombinasi Kemometrik

Abstrak

VCO merupakan salah satu minyak nabati yang memiliki banyak manfaat untuk kesehatan dan industri kosmetik, tetapi harganya relatif tinggi dibandingkan dengan minyak nabati lain, sehingga rentan terjadi pemalsuan minyak. Spektrofotometri UV-Vis dan kombinasi kemometrik dikembangkan untuk membedakan VCO dengan minyak lainnya. Minyak kedelai (SO) dan minyak bunga matahari (SFO) merupakan bahan pemalsuan utama VCO. Penelitian ini bertujuan untuk mengetahui kemampuan metode spektrofotometri UV-Vis kombinasi kemometrik untuk membedakan VCO dengan SO dan SFO. Sampel diukur serapannya pada panjang gelombang 200–400 nm. Data spektrum UV-Vis dianalisis lebih lanjut menggunakan kemometrik PCA dan HCA untuk mengklasifikasikan sampel. Model PCA yang dibuat dapat membedakan VCO, SO, dan SFO menggunakan *software* RStudio 4.4.2 dengan sebaran variasi data sebesar 81,3% untuk PC1 dan 17,1% untuk PC2. Sampel VCO terlihat memisah dari sampel lainnya, sementara SO dan SFO 100% terletak berdekatan karena sifat fisikokimianya yang mirip. Sampel campuran minyak mengelompok sesuai komposisi campurannya. Dalam analisis HCA juga terlihat adanya pengelompokan sampel yang sama seperti dalam analisis PCA. Spektrofotometri UV-Vis kombinasi kemometrik sudah dapat digunakan untuk membedakan VCO dengan SO dan SFO.

Kata Kunci: minyak kelapa murni, spektrofotometri UV-Vis, kemometrik

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1. Introduction

VCO is produced from fresh, ripe coconut meat using mechanical or natural methods, with little or no heat, so that it retains its natural components and is potentially more beneficial than coconut oil.¹ VCO has a distinctive aroma because it still contains natural phytonutrients, namely high levels of tocopherol (vitamin E).^{2,3} In addition to having antiviral and antibacterial activity, VCO is useful in the cosmetics industry as a moisturizer, soap, and shampoo.⁴ Economically, VCO has a higher selling price than other vegetable oils, making it susceptible to fraud and adulteration, which can affect the quality and purity of a product.^{5,6} The most common vegetable oil adulteration is the mixing process with cheaper vegetable oils or non-edible oils.⁵ The main adulteration materials for VCO are soybean oil (SO), sunflower oil (SFO), coconut oil (CO), mustard oil (MO), paraffin oil, and palm oil (PO).^{7,8} Vegetable oil contains tocopherol as one of the main components. In addition, vegetable oil also contains components in the form of phospholipids, sterols, and carotenoids, all of which have chromophore groups that absorb at UV-Vis wavelengths.⁹ VCO has UV absorption at wavelengths of 200 nm to 300 nm.¹⁰ Meanwhile, SO has UV absorption at wavelengths of 230-310 nm. SO presents main peaks at 232, 255, 265, and 270 nm and two small peaks in the region of 290 and 310 nm.¹¹ While SFO presents the main peaks at 232 and 270 nm.¹² The mixture of oils can cause overlapping because the components in the oil absorb at the same or adjacent wavelengths, making them difficult to detect visually. Therefore, a chemometric method is needed to extract information from the sample.¹³ Chemometric methods commonly used for the analysis of vegetable oil adulteration are PCA (principal component analysis) and HCA (hierarchical cluster analysis). PCA and HCA have been used to analyze the adulteration of genuine extra virgin olive oil (EVOO) with canola oil, sunflower oil, corn oil, and soybean oil, with results indicating that the oil mixtures can be separated into three main components.¹⁴

Analysis of virgin coconut oil (VCO) adulteration has been widely conducted using instrumental techniques such as ATR-FTIR combined with chemometrics. Furthermore, NMR, Near Infrared Spectroscopy (NIR), and Electrospray Ionization Mass Spectrometry (ESI-MS) methods have proven effective in distinguishing VCO from other vegetable oils through more comprehensive chemical profiling.^{5,8,14}

Furthermore, UV-Vis spectroscopy is being developed as an alternative analytical method that is simpler, faster, and relatively low-cost. The combination of UV-Vis spectroscopy with multivariate analysis, such as PCA and HCA, has been reported to group and identify

differences among oil samples based on their spectral characteristics. Analysis of VCO adulteration with SO and SFO using combined UV-Vis spectrophotometry and chemometrics has never been carried out. Therefore, in this study, UV-Vis spectrophotometry combined with PCA and HCA chemometrics was chosen to assess VCO purity because it enables rapid identification of compounds and facilitates visualization of data grouping across samples.^{15,16}

2. Materials and Method

2.1. Tools

The tools used in this study were beakers (100 mL beaker, 25 mL volumetric flask, 10 mL measuring flask), a UV-Vis spectrophotometer (Shimadzu UV1780, Japan) with UV Probe 2.70 software, a vortex, a micropipette (Dragon OneMed, China), and RStudio 4.4.2 software.

2.2. Materials

Certified virgin coconut oil, soybean oil, and sunflower oil, n-hexane pa (Merck).

2.3. Methods

2.3.1. Sampling

Samples of virgin coconut oil, soybean oil, and sunflower oil were purchased from PT Syailendra Bumi Investama Karanganyar, provided with certificate of analysis (COA).

2.3.2. Organoleptic Test

Organoleptic tests are carried out by at least 3 panelists or 1 expert.¹⁷ Testing was carried out with a 1×24-hour washout period to ensure that the effects of previous treatment do not affect the results of the next treatment.¹⁸ In addition, organoleptic tests were carried out using the inclusion and exclusion criteria listed in Table 1.

2.3.3. Measurement of the Absorbance of VCO, SO, and SFO

The VCO sample was transferred into a 10 mL measuring flask to a volume of 200 μ L and diluted with n-hexane to the limit mark to obtain a stock solution at a 50x dilution. After that, 1000 μ L of the stock solution was transferred to a 10 mL measuring flask, resulting in a 500x dilution. SO and SFO samples were taken, up to 20 μ L each, into a 25 mL measuring flask and diluted with n-hexane to the limit mark to obtain a stock solution at a 1250x dilution. The SO stock solution was brought

Table 1. Inclusion and exclusion criteria

Category	Criteria
Inclusion	<ol style="list-style-type: none"> 1. Willing to participate in organoleptic quality testing by signing an informed consent 2. Have no history of food allergies 3. Do not consume or smell foods that have a strong taste or smell within 6 hours before testing. 4. Not colorblind 5. Physically and mentally healthy 6. Do not use cosmetics such as perfume and lipstick 7. Do not smell anything with a strong odor within 6 hours before testing.
Exclusion	<ol style="list-style-type: none"> 1. Experiencing a sick condition when organoleptic analysis is to be carried out, which can affect the function of the senses of sight, taste and smell 2. Allergy to an ingredient in the product being tested 3. Taking medications that can affect the senses of sight, taste, and smell 4. Exit the study before completing a complete organoleptic analysis

up to 625 μL in a 10 mL measuring flask, yielding a final dilution of 20,000x. Meanwhile, 313 μL of SFO stock solution was transferred to a 10 mL measuring flask, yielding a final dilution of 40,000x. Furthermore, the solution was measured for its absorbance using UV-Vis spectrophotometry (Shimadzu UV-1780, Japan) with UV Probe 2.70 at wavelengths of 200-400 nm.

2.3.4. Preparation and Measurement of the Absorbance of Oil Mixtures as Adulterants

The absorbance of the oil mixture prepared according to Table 2 was measured using UV-Vis spectrophotometry (Shimadzu UV-1780, Japan) with the UV Probe 2.70 software in the wavelength range of 200-400 nm.

2.3.5. Chemometric Analysis

Multivariate data analysis was performed using RStudio 4.4.2. Data obtained from absorbance measurements using UV-Vis spectrophotometry were analyzed using PCA (principal component analysis) and HCA (hierarchical cluster analysis). Before being used for chemometric analysis, UV-Vis spectrum data

needs to be pretreated to minimize baseline variations, noise, and light scattering.^{5,19}

3. Result

3.1. Sample Characteristics

VCO, SO, and SFO have been characterized through organoleptic tests, namely color, odor, and taste, in accordance with the Indonesian National Standard¹⁷ and are declared to meet the requirements. The results of the organoleptic test are shown in Table 3.

The results of organoleptic observations of VCO by panelists are in accordance with the Indonesian National Standard.¹⁷ The clear color of VCO is caused by the manufacturing process, which uses very low heating or no heating and without chemical processes.²⁰ Coconut oil produced by the dry method has good quality, clear color, clean, and fragrant aroma.²¹ In this study, the extraction method used was cold pressed, which is a dry method. The results of organoleptic observations of SO by panelists are in accordance with the Indonesian National Standard.²² The unpleasant odor in soybean oil appears due to the

Table 2. Mixing ratio of vegetable oil as an adulterant

Code	Volume taken (mL)		
	VCO	SO	SFO
SO28	3.6	1.4	0
SO48	2.6	2.4	0
SO62	1.9	3.1	0
SO74	1.3	3.7	0
SFO28	3.6	0	1.4
SFO48	2.6	0	2.4
SFO 62	1.9	0	3.1
SFO74	1.3	0	3.7
SO16SFO68	0.8	0.8	3.4
SO32SFO4	3.2	1.6	0.2
SO34SFO34	1.7	1.7	1.7
SO68SFO16	0.8	3.4	0.8

Table 3. Organoleptic Test of Virgin Coconut Oil.17

Organoleptic Test	Organoleptic test results	
	Observation result	Test requirements (SNI)
VCO		
Color	Clear	Colorless to pale yellow
Smell	Coconut oil specialties	Fresh coconut specialties
Flavor	Coconut oil specialties	Normal
SO		
Color	Clear yellowish	Yellow
Smell	Almost odorless	Normal
Flavor	Typical weak soybean oil	Normal
SFO		
Color	Clear yellowish	Normal
Smell	Odorless	Normal
Flavor	Tasteless	Normal

activity of the lipoxygenase enzyme in soybean seeds, which produces ethyl phenyl ketone, which causes the distinctive aroma of soybeans and unpleasant taste.²³ The panelists' organoleptic observations of sunflower oil are in accordance with Indonesian National Standards.²⁴ According to research, sunflower oil contains more carotenoid pigments of the lutein and zeaxanthin types, which give it a yellow-to-faint-orange color.¹²

3.2. Oil Spectrum Profile

Figure 1A shows an overlay of the spectra results of 100% VCO, SO, and SFO oils, while Figure 1B shows an overlay of the results of the oil mixture using UV-Vis spectrophotometry.

Based on the measurement results in Figure 1A, virgin coconut oil exhibits an absorption peak at 219 nm. Virgin coconut oil contains lauric acid, caprylic acid, and myristic acid as the main components. These three fatty acids contain a carboxyl group (-COOH), which serves as an auxochrome and can absorb light at short

wavelengths (200–215 nm). This absorption is related to the $n \rightarrow \pi^*$ electron transition or a higher energy transition but occurs with low intensity. Therefore, virgin coconut oil does not show significant absorption at wavelengths above 250 nm.²³

In addition, virgin coconut oil also contains oleic acid and linoleic acid, although in small percentages, namely 10% and 2.5%, respectively. Linoleic acid and oleic acid have chromophore groups, so the combination of auxochrome and chromophore provides absorption at a lower energy level, which is related to the electron transition $\pi \rightarrow \pi^*$.²³

The difference in absorbance profiles between coconut oil and soybean oil and sunflower oil is caused by differences in carbon chain saturation in their constituent fatty acids. Linoleic acid, as a polyunsaturated fatty acid, has double bonds capable of forming a conjugated diene system that functions as an effective chromophore. In Lipid Oxidation, the presence of this conjugated π system lowers the transition energy gap between the HOMO and

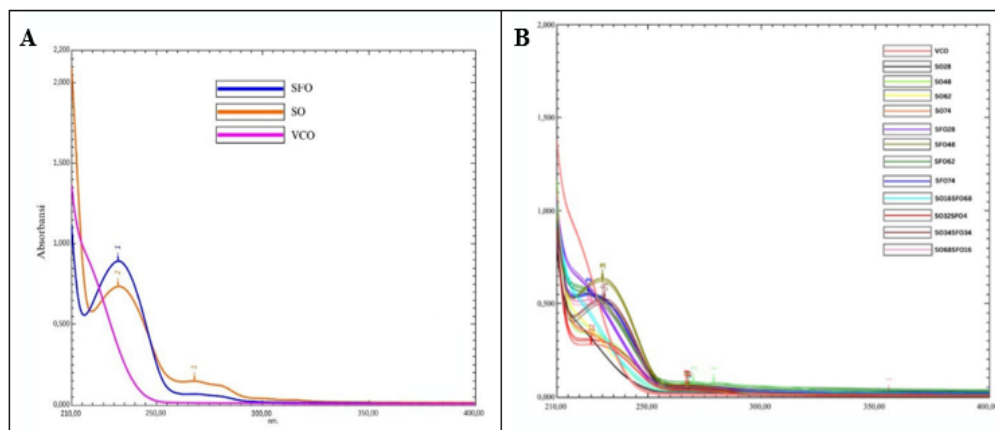


Figure 1. Spectral profiles of pure oil (A) and oil mixtures (B)

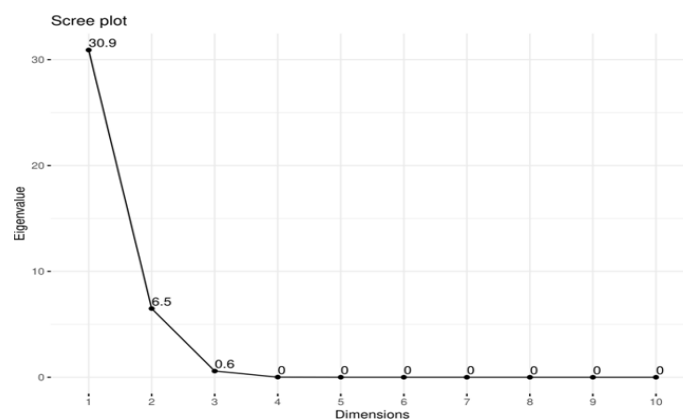


Figure 2. Results of the scree plot curve

LUMO orbitals, thus allowing significant absorption of electromagnetic radiation at a wavelength of 232 nm. In contrast, lauric acid, which is a saturated fatty acid, does not have a π electron system and only has an auxochrome group, so the energy required for electron excitation is beyond the detection range of conventional UV-Vis spectrophotometry, resulting in no significant absorption peak.¹¹

Soybean oil gives absorption peaks at wavelengths of 232 nm and 268 nm. According to research that has been conducted, soybean oil has UV absorption at a wavelength of 230-310 nm. Soybean oil presents main peaks at 232, 255, 265, and 270 nm and two small peaks in the region of 290 and 310 nm.¹¹ While sunflower oil provides absorption peaks at wavelengths of 232 and 268 nm. Other studies state that SFO has main peaks at 232 and 270 nm.¹³ The absorption peak at a wavelength of 232 nm indicates that linoleic acid, a major component of soybean and sunflower oils, has begun to undergo structural changes due to oxidation. This change is characterized by the formation of conjugated dienes, a condition in which the double bonds in the fatty acid molecule shift closer together. Technically, this new structure allows electrons to more easily move from a lower energy level (HOMO) to a higher energy level (LUMO) by absorbing light precisely at 232 nm.¹¹ The results of these measurements are shown in Figure 1A.

Based on the measurements in Figure 1B using UV-Vis spectrophotometry, the spectrum profiles of virgin coconut oil samples and adulterated oil mixtures show varying intensities. The spectrum profile of the oil mixture shows results that are not significantly different from those of pure coconut oil, soybean oil, and 100% pure sunflower oil.

At wavelengths of 219-250 nm, there is typical absorption similar to that of 100% virgin coconut oil, but only in intensity. This typical absorption is observed in a mixture of oils with the ratios SO28, SO48,

SO62, SO74, SFO28, SO32SFO4, and SO68SFO16. Meanwhile, a mixture of oils with a ratio of SFO48, SFO62, SFO74, SO16SFO68, and SO34SFO34 does not show the typical absorption of 100% virgin coconut oil because the content of virgin coconut oil is lower. The mixture of oils used does not consist only of 100% soybean oil; it also contains 100% virgin coconut oil and sunflower oil, according to the formula. Therefore, the composition of the sample affects the shape of the resulting spectrum.

3.3. Principal Component Analysis (PCA)

3.3.1. Scree Plot Result

The results of the Scree Plot in Figure 2 show the 2 highest eigenvalues, namely 30.9 and 6.5, with cumulative diversity values of 81.3% and 17.1%, respectively. The total of the two cumulative diversity values is 98.4%.

Based on the Kaiser criterion, an eigenvalue greater than 1 indicates an informative PC.^{23,25} In addition, the graphic visualization also shows that the model with two PCs already presents the data well, so that PC3 is not needed. The analysis shows that the first two PCs have eigenvalues >1 , namely PC1 of 81.3% and PC2 of 17.1%, with a total cumulative diversity of 98.4%. Because the amount of variation explained by PC1 and PC2 exceeds 70%, the principal component diagram provides a good two-dimensional representation.^{26,27}

3.3.2. Score Plot Results

Figure 4A shows the results of the score plot curve, while Figure 4b shows the results of the dendrogram using R Studio 4.4.2 software. Based on the PCA results in RStudio, the score plot in Figure 3A shows separation of samples by oil mixture concentration.

Based on Figure 3A, VCO 100% is separated from the oil mixture group, SO, and SFO 100%, while SO

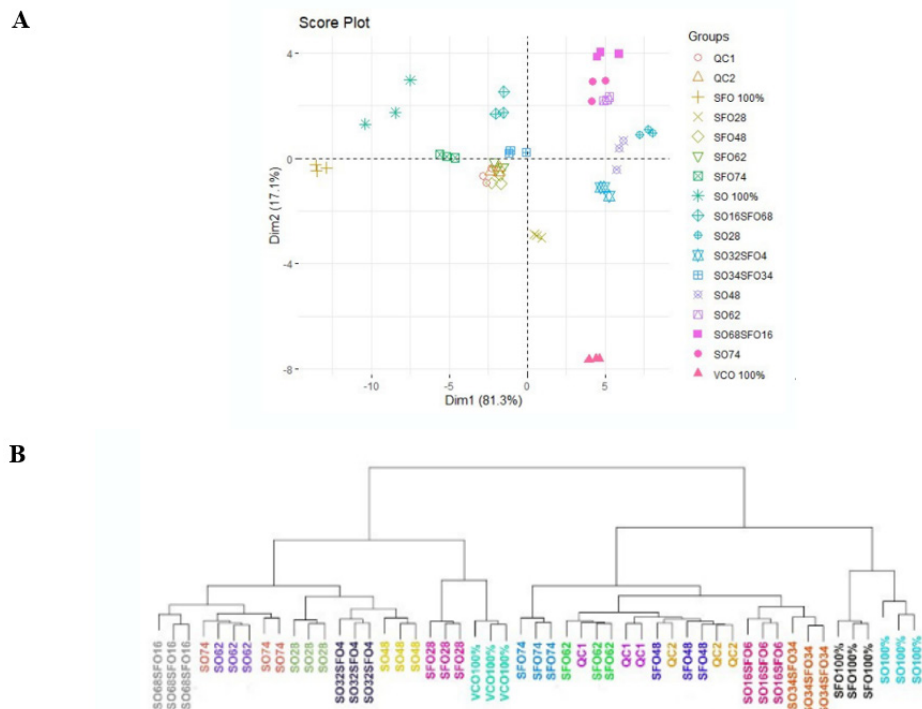


Figure 3. (A) Score plot and (B) dendrogram visualization with R Studio

and SFO are on adjacent plots, possibly due to similar physicochemical properties.²⁶ The distance between samples indicates the level of similarity between samples. The farther apart the samples are, the less similar they are.

The mixed oil samples containing virgin coconut oil and soybean oil are separated from the oil mixture containing virgin coconut oil and sunflower oil, but they appear to be clustered in the same area based on the composition of the oil mixture. The soybean oil mixture samples are spread between virgin coconut oil and 100% soybean oil. While the sunflower oil mixture samples are spread between virgin coconut oil and 100% sunflower oil. The more a certain oil composition is in a sample, the closer the sample's position is to that oil. For example, a sample of a mixture of oils with an SFO28-to-SO32SFO4 ratio is closer to 100% pure coconut oil. This is because the component that is present in greater quantity is 100% pure coconut oil. While for samples QC1 and QC2, they appear close together and clustered in the same area. Thus, the PCA model created can be used to differentiate groups of oil mixtures, pure coconut oil, soybean oil, and 100% sunflower oil.

Based on the dendrogram in Figure 3B, the HCA analysis produced two large clusters. The two clusters are cluster groups containing 100% virgin coconut oil samples and a mixture of virgin coconut oil and soybean oil, and clusters containing all 100% soybean oil samples, 100% sunflower oil, a mixture of virgin coconut oil and sunflower oil, and QC samples.

The first cluster in Figure 3B comprises 100% virgin coconut oil and a mixture of virgin coconut oil and soybean oil. In this arm, there are samples of a mixture of oils in the ratios SO68SFO16, SO74, SO62, SO28, SO32SFO4, and SO48. In the next arm, there is a mixture of oils with an SFO28-to-100 % virgin coconut oil ratio. These results are in accordance with the results of the PCA analysis. In the second cluster, there are samples of a mixture of oils with a ratio of SFO74, SFO62, QC1, SFO48, QC2, SO16SFO6, SO34SFO34, 100% sunflower oil, and 100% soybean oil. These results are in accordance with the results of the PCA analysis. Based on the results of the HCA analysis carried out in the wavelength range of 218-255 nm using UV-Vis spectrum data in RStudio, the samples show a fairly clear grouping by oil component.

4. Discussion

Virgin coconut oil is one of the vegetable oils with many benefits, including antiviral, antibacterial, and antioxidant properties.^{2,3} To ensure the quality of the oil used in this study, characterization was carried out according to the requirements of Standar Nasional Indonesia.¹⁷ Organoleptic tests are conducted by at least 3 panelists or 1 expert, with inclusion and exclusion criteria, to ensure the research results are objective and representative. The selection of panelists for organoleptic testing was conducted according to the set inclusion and exclusion criteria, and panelists were required to complete an informed consent form before participating in the test. Organoleptic testing of color, odor, and taste began with pure coconut

oil, followed by a 1×24-hour washout period, then continued with testing on soybean oil and sunflower oil to the Indonesian National Standard. Testing is done by transferring the oil sample into a test tube and then observing it with the eyes. Washout period, which is a rest period given to ensure that the effects of the previous treatment do not affect the results of the next treatment.¹⁸ For the odor test, the oil sample is smelled at a distance of approximately 5 cm from the nose, then shaken towards the nose to determine the smell. Taste testing is done by pouring the oil sample into a clean teaspoon and tasting it with the tongue. The results showed that the vegetable oil used met all the requirements.

Virgin coconut oil has a clear appearance and a distinctive fresh-coconut smell, while soybean and sunflower oils have a clear yellowish appearance and are almost odorless. When mixed, the difference between virgin coconut oil, soybean oil, and sunflower oil cannot be distinguished in terms of color. In addition, virgin coconut oil, soybean oil, and sunflower oil have close wavelengths. The wavelength range is 219-268 nm.

Pure vegetable oil is oil without any mixture or contamination from other oils. The three oils share overlapping spectral patterns, making them difficult to distinguish visually and potentially leading to counterfeiting or fraud. Therefore, additional analysis using UV-Vis spectrophotometry is needed to analyze the counterfeiting of virgin coconut oil.

Based on previous research, UV-Vis spectrophotometry can be used to analyze olive oil adulteration with soybean oil, canola oil, and corn oil at different concentrations, namely 1.5, 10, 20, 50, 70, and 90% (v/v) for each oil, at a wavelength of 456 nm.²⁸ In addition, UV-Vis spectroscopy can be used for the analysis of adulteration of extra virgin olive oil with sunflower oil and corn oil with different concentrations, namely 0.5, 15, 25 and 100% w/w. The results showed that sunflower oil and corn oil were detected by UV absorption at 270 nm and 232 nm.²⁹ The UV-Vis spectrum results of pure oil are in the adjacent wavelength range. In addition, the UV-Vis spectrum results of the oil mixture obtained are difficult to classify visually, so further analysis is needed to identify pure coconut oil, soybean oil, and sunflower oil using chemometric techniques.

The combination of UV-Vis spectrophotometry and chemometrics has been widely used for the identification, discrimination, and authentication of medicinal plants. In this study, the well-known *Principal Component Analysis* (PCA) chemometric analysis was chosen to predict sample adulteration with appropriate

precision and sensitivity.²⁸ PCA has been used to detect adulteration of olive oil with cheaper vegetable oils and to analyze traditional herbal medicines.³⁰

PCA is a multivariate data reduction technique that uses linear transformations to create new variables called principal components (PCs). Generally, the first two PCs are used to create a PCA plot because they capture most of the variation in the data. The pattern recognized in this study is the absorbance (absorption) value for each test sample. PCA will recognize this pattern and group virgin coconut oil, soybean oil, and sunflower oil based on their variable similarities.¹⁹

UV-Vis spectrum needs to be pre-treated before being analyzed chemometrically. This study uses a pre-treatment technique, namely smoothing. Spectral smoothing was first applied to reduce high-frequency noise without distorting the original spectral pattern. The smoothed spectra were then subjected to wavelength selection to remove spectral regions with excessive noise and low analytical relevance. This step was essential to retain wavelength ranges that provide the most significant absorption information, representing the overall characteristics of the samples. Furthermore, data normalization was performed using RStudio's autoscaling method. Autoscaling was conducted column-wise by mean-centering each wavelength variable, then dividing by its standard deviation, resulting in variables with zero mean and unit variance. This preprocessing step ensured equal contribution of all wavelengths in the subsequent PCA and HCA models and prevented variables with higher absorbance intensity from dominating the analysis.^{19, 32}

Based on the spectrum profile in Figure 1, all samples exhibit significant absorbance in the 210-250 nm range. At wavelengths of 250-400 nm, there is almost no significant absorbance. Virgin coconut oil gives an absorption peak at a wavelength of 219 nm. Soybean oil exhibits absorption peaks at wavelengths of 232 nm and 268 nm. Sunflower oil exhibits absorption peaks at wavelengths of 232 nm and 268 nm. Wavelengths of 200-210 nm are better excluded to produce good data. Therefore, the wavelength range chosen for PCA analysis, namely 218-255 nm, gives a significant absorbance value. In addition, HCA (Hierarchical Cluster Analysis) is a chemometric technique often used to analyze fatty acids in vegetable oils. HCA is a chemometric analysis that uses a dendrogram (a two-dimensional plot) to identify the distance between samples and datasets.¹⁶ HCA groups data into several clusters based on their level of similarity.

In the first stage, distance calculations are performed to determine the level of similarity between objects. The most similar objects (the closest distance) will be

grouped into one cluster, while dissimilar objects will be separated into different clusters. Furthermore, in the second stage, the small clusters formed are combined into larger clusters.³² Based on HCA analysis of UV-Vis spectra using RStudio, a fairly clear grouping of samples was observed by component. The HCA is used to group oil samples based on their chemical properties. Through this approach, genuine and adulterated oil samples tend to form separate groups. This separation makes it easier to detect adulteration both visually and through statistical analysis.¹⁶

In this study, we deliberately utilized PCA and HCA to determine whether the natural spectral variances, driven by the intrinsic chromophores of VCO, soybean, and sunflower oils, were sufficient to distinguish the samples without the bias of pre-defined labels. By opting for an unsupervised approach, we aimed to demonstrate the inherent 'chemical fingerprint' of these oils while avoiding the potential for overfitting, which is a common risk in supervised models like PLS-DA when working with specific sample sizes. Thus, this work establishes a necessary diagnostic foundation, proving that the spectral data is naturally discriminative before proceeding to more complex predictive algorithms.

5. Conclusion

Based on the results of this study, the combination of UV-Vis spectrophotometry with principal component analysis and hierarchical cluster analysis chemometrics can be used to distinguish between VCO mixtures containing SO and SFO.

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Conflict of Interest

The authors declare no conflicts of interest.

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