Machine Learning Techniques for Predicting Olive Oil Pigment Concentrations

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Abstract. This study presents optimization and machine learning (ML) methods for predicting pigment concentrations in Extra Virgin Olive Oil (EVOO) using UV-Vis spectroscopy data and compares them to the standard deconvolution approach. We tested three EVOO samples: standard, fresh, and Monocultivar Frantoio. All methods demonstrated great spectrum reconstruction accuracy of $R^2 > 0.99$. The optimization technique, which employed Non-Negative Least Squares (NNLS) and Limited-memory Broyden-Fletcher-Goldfarb-Shanno with Bounds (L-BFGS-B) algorithms, consistently yielded non-negative pigment concentration predictions. Both new methods predicted higher total pigment concentrations than the traditional method, with differences ranging from 2.124 mg/kg (Fresh EVOO) to 7.329 mg/kg (Monocultivar Frantoio). However, there are still issues in reliably quantifying trace pigments, with all approaches displaying variations when predicting very low amounts. This comparison provides valuable insights on EVOO quality assessment and authentication methodologies. Our methodology is a viable alternative analytical method for EVOO analysis, with the potential to improve the reliability and application of pigment quantification in both research and industrial settings.

Keywords: Pigment Analysis, Spectral Deconvolution, Machine Learning, EVOO, UV-Vis Spectroscopy, Food Science

1 Introduction

EVOO is a highly valued product recognized for its unique flavor profile and plenty of health advantages. Sieved from the olive tree (Olea europaea L.), an antiquity cultivation in Mediterranean area, EVOO is considered as one of tastiest Olive oil's due to its superb features compared with mild ones including acidity levels less than 0.8% and a sensory score above 6.5 [1]. The authenticity and quality of EVOO is significantly affected by the presence of chlorophylls and carotenoids, constituting the majority of pigment content [2]. Lutein, beta-carotene, violaxanthin, and neoxanthin are the main pigments found in EVOO, along with a variety of lesser derivatives, which are impacted by the olive cultivar, fruit ripeness, production techniques, and storage [3-6].The traditional methods for the determination of pigments in EVOOs like spectral deconvolution and High Performance Liquid Chromatography (HPLC) can be inaccurate, costly and time consuming [7]. These procedures often include chemical extraction and

chromatography which can alter the oil's constitution [8]. UV-Vis spectroscopy has been emerged as a non-destructive alternative for pigments analysis in EVOO, particularly through recent surface science advancements [9]. Accurately measuring individual pigment concentrations is challenging due to the complex EVOO spectra, with overlapping absorbance signals from different pigments [10]. In this context, introducing new computational methods for data analysis in spectroscopic techniques in food science would be a great improvement [11–12], leading researchers to explore advanced models based on ML algorithms and optimization processes. These approaches have shown great potential for handling big data and improving the accuracy and efficiency of analytical processes across various scientific disciplines [13]. This research advances these efforts by applying ML to UV-Vis spectroscopy data to enhance pigment concentration predictions in EVOO. The study evaluates various ML models, comparing their effectiveness with traditional spectral deconvolution, and assesses the feasibility of ML techniques for rapid, non-invasive pigment analysis in quality control and authenticity verification of EVOO.

2 Background

2.1 Spectroscopic Methods in EVOO Analysis

Simple spectrophotometric techniques are low accuracy and time-consuming in the study of pigments colored compounds present brown-red EVOO samples, whereas traditional methods like HPLC may it involve uncertain results considering peculiar matrix complexity [7]. So scientists have looked into several non-destructive spectroscopic methods for the analysis of pigments in EVOO. To ascertain the pigment concentrations in virgin and EVOO, Borello and Domenici [13] compared two near UV-Vis spectroscopic methods. The entire absorption spectrum was analyzed using a mathematical deconvolution approach, and found more accurate and consistent pigment concentrations than conventional method that relied on absorbance values at wavelengths. They noted limitations in detecting minute pigment and analyzing fresh olive oils. Using a mathematical analysis of near UV-visible absorption spectra, Lazzerini and Domenici [14] expanded on this work by examining pigment concentrations in EVOOs made in Tuscany, Italy. Using their method, four main pigments (lutein, β-carotene, pheophytin A, and pheophytin B) could be measured. With total pigment concentrations ranging from 6.65 ppm to 27.58 ppm, the study found significant variations in pigment profiles across different harvesting years. A digital tool called EVOODec was created by Jurinovich and Domenici [20] to analyze the UV-Vis spectra of EVOOs without the need for chemical treatment. With an average user understanding score of 7.6 out of 10, this tool showed promise for accessible pigment analysis in educational settings.

2.2 ML Applications in EVOO Quality Assessment

The use of spectroscopic data comined with ML methods has significantly improved the effectiveness and precision of pigment analysis in EVOO. Venturini et al. [11]

explored a small, affordable fluorescence sensor paired with various ML techniques to evaluate the quality of EVOO. Their research illustrated how ML can accurately assess oil quality without extensive pre-processing, utilizing random forests (RF) and artificial neural networks (ANN) models, achieving complete classification accuracy. Gyftokostas et al. [19] employed Linear Discriminant Analysis (LDA), Gradient Boosting, and spectroscopic data to classify Greek EVOOs based on their cultivar origin. Their Gradient Boosting model, using Laser-Induced Breakdown Spectroscopy (LIBS) data, reached a training accuracy of 96.0% and an external validation accuracy of 93.8%. Additionally, Gucciardi et al. [25] proposed a new approach for evaluating the quality of olive oil. It paired a small optical fluorescence sensor with ANNs. Among the neural network architectures they investigated, the conditional convolutional neural network (Cond-CNN) outperformed the others with an accuracy of 82% in oil classification.

UHPLC-HRMS, or ultra-HPLC coupled with high-resolution mass spectrometry, was used by Arrizabalaga-Larrañaga et al. [22] to perform a thorough investigation on the pigment profiles of Spanish EVOO. Their research has revealed significant differences in total pigment content across different regions of Spain. The changes in virgin olive oil during storage were observed by Lobo-Prieto et al. [21] using fluorescence spectroscopy in conjunction with parallel factor analysis (PARAFAC). The study showcased the potential of fluorescence-based methods for pigment analysis by demonstrating high correlation coefficients (0.98) between pheophytin concentration measured by HPLC and fluorescence data. Despite significant advancement in EVOO pigment analysis, several challenges remain such as detecting minute pigment, developing robust models that account for variation in chemical properties among samples and integrating multiple analytical methods for comprehensive quality assessment. According to numerous studies, potential avenues for future research include:

1. Improving predictive models for olive oil authenticity and categorisation by incorporating cutting-edge ML and deep learning approaches [19, 25].
2. Creating on-the-spot, real-time analysis techniques for quick quality evaluation [11, 16].
3. Investigating how spectroscopic data might be integrated with other chemical and sensory characteristics to provide a thorough assessment of quality [21, 22].

Integrating advanced data analysis techniques, such as ML with spectroscopic techniques presents significant potential for improving the quantification of EVOO pigments. These advancements could greatly influence quality control practices and enhance consumer trust in EVOO products. Our research builds on this foundation, aiming to advance the field through innovative ML and optimization techniques.

3 Materials and Methods

3.1 Data Collection and Spectral Acquisition

UV-Vis spectroscopy data collected from a range of EVOO samples, including commercially available and freshly squeezed oils, were used in this investigation. Jurinovich and Domenici (2022) [20] were the first to publish the dataset. Three different kinds of EVOO samples were examined: Standard EVOO, Fresh EVOO and Monocultivar Frantoio EVOO. Using a spectrophotometer capable of measuring in the 380–720 nm range, UV-Vis absorbance spectra were acquired with a spectral resolution of 1 nm. Using this wavelength range, the absorption characteristics of the main pigments in olive oil, including carotenoids, pheophytins, and chlorophylls, were captured [9, 10]. As suggested by Borello and Domenici [13], oil samples were filtered prior to spectral capture to guarantee clarity and reduce light scattering effects. At room temperature, absorbance readings were recorded using a quartz cuvette with a 1 cm path length. Air was used as a reference to calibrate the spectrophotometer. A total of 341 data points, spanning the whole 380–720 nm range, were acquired for each sample. The spectral data was stored in CSV format, where the wavelength (nm) and associated absorbance (a.u.) values were shown in two columns. Based on their importance in the composition of EVOO, the pigments taken into consideration in this study were [2, 4]: Phenophytin a (Pheo-a), Chlorophyll b (Chl-b), β-carotene (b-CAR), Lutein (LUT), Neoxanthin (NEX), Chlorophyll a (Chl-a), and Phenophytin b (Pheo-b). Triolein (TRIO) was also added to symbolize the EVOO matrix, which is mainly made up of triglycerides and fatty acids [10]. In the spectrum analysis and ML model creation that followed, reference data encompassing the same wavelength range (380-720 nm) for the molar extinction coefficients of these pigments was used. This extensive dataset served as the basis for the development and assessment of our ML models for pigment concentration prediction as well as a thorough examination of the pigment composition in a variety of oil samples.

3.2 Data Preprocessing

Data preprocessing is crucial for spectral analysis and ML applications in EVOO pigment quantification. A critical step involves aligning EVOO sample data with pigment reference data to compare absorbance and extinction coefficient values at the same wavelengths. We then normalize extinction coefficients to account for scale differences between pigments. To enhance data quality, we apply a Savitzky-Golay filter for spectral smoothing, reducing noise while preserving underlying spectral features [26]. The Savitzky-Golay filter can be expressed as:

$$y_i^* = \sum_{n=-m}^{m} c_n y_{i+n} \tag{1}$$

where (y_i^*) is the smoothed value, (y_i) is the original data point, (c_n) are the filter coefficients, and $(2\mathrm{m} + 1)$ is the window size. For ML models, we implement standard scaling of input features to ensure all variables are on a similar scale. We perform

validation tests at several stages of the preprocessing pipeline to guarantee data consistency and integrity, which is necessary for trustworthy analysis in the future. With this thorough approach, we can accurately anticipate pigment concentration and establish dependable comparisons between analytical methods, as well as prepare our spectrum data for both conventional optimization methods and ML techniques.

3.3 Traditional Deconvolution Method

We used the conventional deconvolution method as outlined by Domenici et al. [10] as a baseline for comparison. Using matrix operations and eigenvector calculations, the full UV-Vis absorption spectrum is analyzed to obtain pigment amounts.

Method 1 Traditional Deconvolution Method

1: Compute overlap matrix of reference spectra
2: Diagonalize overlap matrix
3: Compute eigenvectors for new base
4: Calculate Spectral Variance (SV) coefficients
5: Compute pigment concentrations
6: Reconstruct spectrum and calculate residuals

In addition to producing the reconstructed spectrum and estimated pigment concentrations, the method calculates residuals. This method makes use of all available spectral information to enable the simultaneous quantification of several pigments. Prior research has demonstrated that the method is accurate [10], but it can be computationally demanding and may have difficulties with extremely complex or noisy spectra.

3.4 Optimization Method

We have implemented an optimization method that makes use of well-established numerical techniques to supplement the conventional deconvolution approach. This approach should yield accurate and useful pigment concentration estimates.

Method 2 Optimization Method

1: NNLS are used to make an initial estimate.
2: L-BFGS-B technique to optimize concentrations
3: Calculate fitted spectrum
4: Compute R-squared and RMSE

This method uses numerical approaches to accurately determine pigment amounts. We start by utilising Non-Negative Least Squares (NNLS) to estimate the pigment concentrations. NNLS ensures that the initial concentrations for pigment analysis are non-negative, which is important from a physical standpoint. The initial guess is refined using the Limited-memory Broyden-Fletcher-Goldfarb-Shanno algorithm with Bounds (L-BFGS-B). The estimation of pigment concentration necessitates optimization issues with bound restrictions, which our approach effectively handles [28]. With the

optimized concentrations, we calculate a fitted spectrum that most closely matches the experimental EVOO spectrum. We compute the coefficient of determination (R-squared) and the Root Mean Square Error (RMSE) to assess the accuracy and fit of the concentration estimates. The optimization procedure is guided by an objective function that minimizes the sum of squared differences between the experimental and fitted absorbance:

$$\min\Sigma(A\_exp - A\_fit)^2 \tag{2}$$

where A_exp is the experimental absorbance and A_fit is the fitted absorbance calculated from the estimated pigment concentrations. This method uses NNLS for initialization and L-BFGS-B for fine-tuning optimization, striking a balance between accuracy and computational efficiency. To ensure that the estimated concentrations remain within physically meaningful ranges, bound constraints are employed during the optimization process.

3.5 ML Methods

To improve our ability to estimate pigment concentration even further, we tested a few ML models. This method seeks to extract intricate linkages from the spectrum data that conventional or optimization approaches might not be able to completely address.

Method 3 ML Method

1: Preprocess and standardize data
2: Train multiple ML models
3: Select best model based on R^2 score
4: Predict concentrations using best model
5: Calculate fitted spectrum
6: Compute R-squared and RMSE

We used a various of ML models to perform spectral deconvolution in our analysis of EVOO samples. Random Forest [29], Gradient Boosting [30], Ridge Regression, K-Nearest Neighbours, and Partial Least Squares Regression are the models we used in our study. When it comes to managing intricate, high-dimensional data, such as spectral information, each of these models has special advantages. We train each ML models on the standardized data. Each model is fitted using the entire dataset. We select the best model based on the R^2 score calculated on smoothed predictions. We use the best-performing model to predict pigment concentrations. We calculate the fitted spectrum using the predicted concentrations.

$$A_{\text{fit}} = \epsilon_{\text{normalized}} \cdot c \tag{3}$$

Where (A_{fit}) is the fitted absorbance spectrum, $(\epsilon_{\text{normalized}})$ is the normalized extinction coefficient matrix and (c) is the vector of predicted concentrations. We compute the R^2 score and Root Mean Square Error (RMSE) to assess the quality of the fit. Complex, non-linear interactions in the spectrum data can be explored with

this ML approach. We can choose the best method for our EVOO pigment prediction task by comparing several models. The robustness and dependability of our predictions are enhanced by the performance measures on smoothed data.

4 Results and Discussion

4.1 Performance Comparison

Using three different approaches—classical deconvolution, optimization, and ML—we examined three EVOO samples: fresh EVOO, standard EVOO, and monocultivar Frantoio. The performance metrics for every method across all samples are compiled in Table 1. Across all samples, all methods demonstrated exceptional spectral reconstruction with high R^2 values (>0.99). In terms of R^2 and RMSE, the Gradient Boosting model routinely beat the optimization method, whereas the traditional method, because of its computational approach, produced the highest R^2 values and least RMSE metrics [10].

Table 1. Performance metrics for each method across EVOO samples

Sample	Method	R^2	RMSE
Standard EVOO	Traditional	0.999042	0.026501
	Optimization	0.995464	0.057675
	Gradient Boosting	0.996166	0.053021
Fresh EVOO	Traditional	0.997805	0.020236
	Optimization	0.993667	0.034375
	Gradient Boosting	0.993966	0.033553
Monocultivar Frantoio	Traditional	0.999350	0.028512
	Optimization	0.995391	0.075958
	Gradient Boosting	0.996044	0.070364

4.2 Spectral Reconstruction

We analyzed the spectral reconstruction capabilities of each method for all three EVOO samples.

Traditional Deconvolution Method.

Fig. 1 show the spectral reconstruction using the traditional method for standard EVOO, fresh EVOO, and Monocultivar Frantoio samples, respectively. The 400–500 nm and 600–700 nm regions, which are crucial for carotenoid and chlorophyll pigments, respectively, were especially well-fitted by the conventional approach for all samples [9]. The best fit (R^2 = 0.999350) was found in the Monocultivar Frantoio sample (Fig. 1), possibly because of its unique pigment profile.

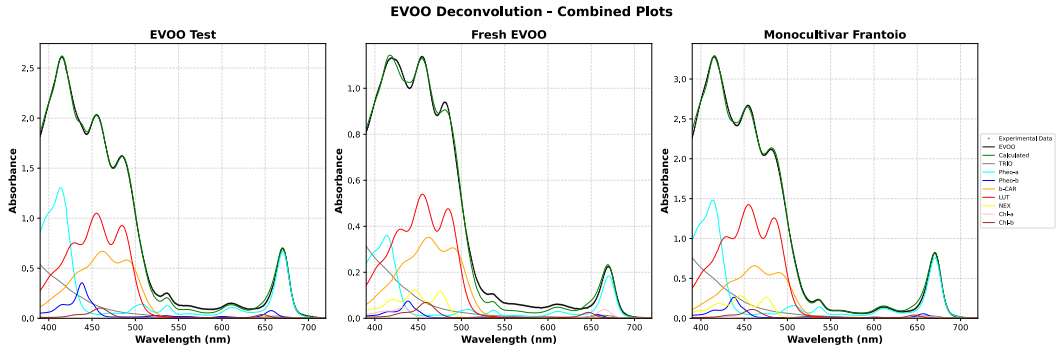

Fig. 1. Spectral reconstruction across EVOO samples using traditional deconvolution method

Optimization Method

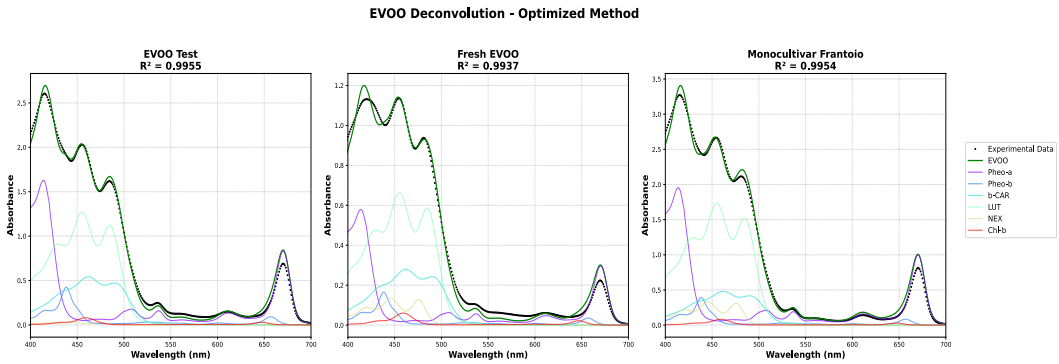

Fig. 2. Spectral reconstruction across EVOO samples using optimization method

The optimization method demonstrated good fits across all samples, with slight deviations in the 450-550 nm range, particularly for the fresh EVOO sample (Fig. 2). This may account for differences in estimated concentrations of carotenoid pigments.

ML Method

For all samples, gradient boosting obtained the highest R^2 values, suggesting that it accounts for the greatest amount of data variance. This implies that it is most successfully capturing the underlying patterns in the spectral data. In addition to consistently generating the lowest RMSE scores, the Gradient Boosting model outperformed the others in terms of predictive accuracy. Thus, the Gradient Boosting model achieved excellent fits across all samples, potentially capturing subtle spectral features that contribute to its improved performance in pigment concentration estimation.

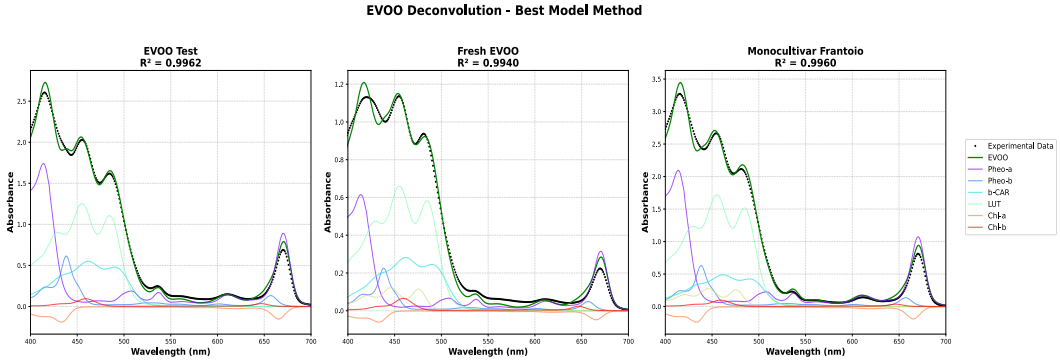

Fig. 3. Spectral reconstruction across EVOO samples using ML method

4.3 Pigment Concentration Predictions

We evaluated each method's predicted pigment concentrations for each of the three EVOO samples. The estimated mg/kg concentrations of the main pigments in each sample are shown in Tables 2.

Table 2. Estimated pigment concentrations (mg/kg)

Samples	Standard EVOO (mg/kg)			Fresh EVOO (mg/kg)			Monocultivar EVOO (mg/kg)		
Pigment	**Traditional**	**Optimi-zation**	**GB**	**Traditional**	**Optimi-zation**	**GB**	**Traditional**	**Optimi-zation**	**GB**
Pheo-a	10.755	13.416	14.348	2.969	4.770	5.068	12.212	16.099	17.270
Pheo-b	1.935	2.320	3.351	0.408	0.903	1.229	1.438	2.136	3.438
b-CAR	2.983	2.415	2.456	1.569	1.244	1.256	2.933	2.137	2.176
LUT	4.953	5.981	5.910	2.545	3.132	3.111	6.723	8.164	8.104
NEX	-0.052	0.162	-0.061	0.647	0.709	0.638	1.478	1.743	1.446
Chl-a	-0.022	0.000	-1.645	0.422	0.000	-0.522	0.216	0.000	-2.074
Chl-b	0.869	0.687	0.801	0.586	0.511	0.552	0.944	0.705	0.838
Total (mg/kg)	**21.421**	**24.980**	**26.865**	**9.146**	**11.270**	**11.853**	**25.944**	**30.984**	**33.273**

4.4 Observations

The traditional method [10] obtained consistent results with the highest R^2 values for all samples. It did, however, occasionally produce negative values when attempting to accurately estimate the concentrations of minor pigments (e.g., NEX and Chl-a in the standard EVOO sample). For all samples, this method estimated the lowest total pigment concentrations. Our optimisation strategy, which combined L-BFGS-B and NNLS, performed better than the conventional approach [28]. It consistently generated

concentration estimates that were not negative and received good R^2 scores for all samples. With variations ranging from 2.124 mg/kg (fresh EVOO) to 5.040 mg/kg (Monocultivar Frantoio), the optimisation method predicted higher total pigment concentrations than the conventional method. Across all samples, the Gradient Boosting model [30] performed better in terms of RMSE and R^2 scores. With estimates that were 5.444 mg/kg (standard EVOO), 2.707 mg/kg (fresh EVOO), and 7.329 mg/kg (Monocultivar Frantoio) higher than those of the conventional method, it calculated the highest total pigment concentrations for all samples. Like the conventional approach, it did, however, occasionally yield negative concentration estimates for trace pigments (such as NEX and Chl-a).

Our results show how novel computational techniques can improve the analysis of EVOO pigments. The optimisation and ML techniques provided enhancements in managing minor pigments and estimating total pigment concentrations, even though all methods displayed high R^2 values, suggesting good spectral reconstruction. Though it needs to be further improved to address problems with negative concentration estimates for trace pigments, the ML approach—in particular, the Gradient Boosting model—shows promise in capturing complex spectral relationships. These findings emphasise the significance of method selection in EVOO pigment analysis and the necessity of carefully interpreting results, especially when it comes to pigments that are present in extremely low concentrations. Future work will focus on improving these models, especially for pigments exhibiting greater differences between methods, and investigating the possibility of combining multiple analytical techniques for more thorough EVOO characterisation.

5 Conclusions

This study compared traditional deconvolution [10], optimization, and ML methods for analyzing pigment concentrations in EVOO using UV-Vis spectroscopy. Our findings demonstrate the potential of advanced computational techniques to enhance EVOO pigment analysis. Across three different EVOO samples, all techniques produced high spectral reconstruction accuracy ($R^2 > 0.99$), confirming their suitability for pigment analysis. A major drawback of the conventional method was addressed by the optimization method, which consistently produced non-negative pigment concentration estimates using the NNLS and L-BFGS-B algorithms [28]. In terms of R^2 and RMSE, the Gradient Boosting model [30] performed better than the other techniques, indicating that ML techniques can effectively capture intricate spectral relationships in EVOO samples. In comparison to the conventional method, both the optimization and ML techniques estimated higher total pigment concentrations, which may suggest improved sensitivity to minor pigments. All techniques were successful in identifying pigment profiles unique to each sample, allowing for the distinction of standard, fresh, and monocultivar Frantoio EVOOs. However, there are still issues with precisely measuring trace pigments, as various approaches have inconsistent results when estimating extremely low concentrations. As shown in other studies [11, 19, 25], these findings emphasize the potential of combining cutting-edge computational methods with

spectroscopic data for EVOO analysis. Although the conventional approach is still useful, optimization and ML techniques have the potential to provide more precise and thorough pigment profiling. Subsequent research ought to concentrate on improving these models, especially regarding trace pigment measurement, and examining how well they work with a larger variety of EVOO samples. Further, combining these spectroscopic techniques with other analytical techniques [21, 22] could result in more reliable tools for EVOO quality evaluation and authentication. Our research demonstrates how advanced computational methods can improve EVOO pigment analysis. These methods have the potential to grow into effective substitutes for current methods in the olive oil industry's quality control and authenticity checks.

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