



Application of chemometrics based on digital image analysis for simultaneous determination of tartrazine and sunset yellow in food samples

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ABSTRACT

Azo dyes, such as tartrazine and sunset yellow, are widely used as affordable and stable food colorants. Accurate quantification is crucial in foods for regulatory monitoring to ensure compliance with safety standards and minimize health risks. This study developed a low-cost and eco-friendly method using digital images and chemometrics for the simultaneous determination of these dyes in food samples. The best prediction results were achieved by applying partial least squares regression to RGB + Grayscale+HSI color histograms, with R^2 of 0.9977, 0.9989, RMSEP of 0.21, 0.10 mg/L and REP of 1.6, 1.0 % for tartrazine and sunset yellow, respectively. The method was successfully applied for determination of tartrazine and sunset yellow in soft drink samples, producing results comparable to those obtained from the HPLC method. This innovative approach provides a practical and reliable alternative for monitoring the dye concentrations, supporting both food manufacturers and health authorities in ensuring compliance with safety standards.

1. Introduction

Artificial food dyes, such as tartrazine (Tar) and sunset yellow (SY), are common azo anionic dyes widely used to enhance the appearance and consumer appeal of various food products (Do Nascimento et al., 2020; Rozamlana et al., 2024; Zhang et al., 2024). Tartrazine, known for providing a bright yellow hue, is the second most commonly used food dye globally. It is especially prevalent in products such as soft drinks, juices, candies, and sauces (Wu & Lee, 2020). Additionally, sunset yellow, which is the third most widely used food dye, is frequently found in sweets, jams, and fermented beverages (Banc et al., 2024; Darabi & Shabani-Nooshabadi, 2021).

Despite their widespread use, overconsumption of these dyes may lead to health issues, particularly in sensitive individuals, causing effects such as allergies, migraines, hyperactivity, and other health concerns (Bakhnooh & Arvand, 2024; Chaudhari et al., 2024; Fan et al., 2024; Wang et al., 2024; Zhang et al., 2025).

For instance, regulations in the European Union (EU) limit the concentrations of tartrazine and sunset yellow in non-alcoholic soft drinks to 100 mg/L and 50 mg/L, respectively, with a total limit of 100 mg/L when used together. Likewise, in the United States (US), the acceptable daily intake (ADI) for tartrazine is 7.5 mg/kg body weight per day, and

for sunset yellow, it is 4 mg/kg body weight per day (EFSA Panel on Food Additives and Nutrient Sources Added to Food, 2009a; EFSA Panel on Food Additives and Nutrient Sources Added to Food, 2009b; EFSA Panel on Food Additives and Nutrient Sources added to Food (ANS), 2014; Rovina et al., 2017; Park et al., 2024; Amchova et al., 2024). To ensure compliance with safety standards, reliable methods for the simultaneous determination of these dyes are crucial (Darabi & Shabani-Nooshabadi, 2021). High-performance liquid chromatography (HPLC) coupled with UV–Vis detection is a standard method for precise dye quantification, known for its high sensitivity and reliability (Agbokponto et al., 2022). However, it is also associated with high costs, the use of toxic solvents, and the need for specialized training and equipment, which suffer environmental, economic, and personal challenges. These obstacles can limit the accessibility of this method. Other techniques, such as electrochemical analysis (Taei et al., 2020), spectrophotometry (Asadollahi et al., 2022), and capillary electrophoresis (Flores-Aguilar et al., 2019), have been used for the simultaneous determination of Tar and SY, but each presents its own limitations in terms of equipment costs, preparation time, and the need for skilled operators (Ostad & Heidari, 2020). Recent advancements in digital imaging and chemometrics offer a promising alternative for dye analysis (Ostad & Heidari, 2020). With the availability of digital devices such as

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smartphones and scanners, digital imaging-based colorimetric analysis method has emerged as a user-friendly, accessible, and non-destructive method suitable for both qualitative and quantitative analysis in food assessment (Choi et al., 2018; Guedes & Pereira, 2019; Santos et al., 2020).

Commercial software such as Adobe Photoshop and MATLAB are widely used for image processing and analysis; however, their high cost and complex training requirements make them less accessible for small labs and independent researchers (Ahmed, 2013; Riedel et al., 2023; Timothy & Forlano, 2019). Photoshop, for example, offers extensive capabilities for digital art creation, drawing, and editing. Though, free alternatives like ImageJ provide a more accessible option, available both as an online applet and a downloadable application, making it a practical solution for those seeking cost-effective tools (Harris-Love et al., 2016; Lin et al., 2023; Timothy & Forlano, 2019).

A digital image is made up of many pixels, each containing three color components—red, green, and blue—known as the RGB color model. Other color models, such as HSI and HSV, are also used (Fiedoruk-Pogrebnik, 2024). Once the image is converted into a color model and numerical data is generated, chemometrics methods can be applied to extract useful information (Ribeiro et al., 2019). Color histograms, which show the distribution of pixel color frequencies, can also serve as input for multivariate analysis.

Digital image analysis combined with chemometrics is a powerful tool for both qualitative and quantitative analysis of food products, including milk, coffee, olive oil, saffron, grape juice, and chicken burgers (Beltrame et al., 2019; De Araújo et al., 2021; De Sousa Fernandes et al., 2019; Dos Santos Pereira et al., 2022; Song et al., 2020). Previous studies have also used chemometrics methods to determine dyes like tartrazine (Vidal et al., 2018) and sunset yellow (Botelho et al., 2014) in foods, with successful applications in candies and soft drinks. Partial least square (PLS) regression is the most popular tool in chemometrics for developing calibration models. PLS algorithm has been successfully combined with spectroscopic (Brereton, 2003, 2007, 2018; Kumar, 2021) and recently digital image analysis (Botelho et al., 2017; Qashqai & Heidari, 2023; Costa et al., 2020; De Sousa Fernandes et al., 2019, De Sousa Fernandes et al., 2019).

This study proposes a digital imaging-based multivariate calibration method for the simultaneous determination of Tar and SY, focusing on three image analysis approaches: color channel analysis, effective color channel analysis, and a color histogram-based analytical system. This innovative method was applied to 10 soft drink samples, and results were validated against the HPLC method to assess its accuracy and applicability in real samples.

2. Materials and methods

2.1. Chemicals

HPLC grade acetonitrile and methanol were purchased from Merck (Merck KGaA, Darmstadt, Germany). Tartrazine and sunset yellow were obtained from Sigma Aldrich (St. Louis, MO, USA). All experiments were carried out at room temperature, using materials of analytical purity grade without further purification. All solutions used in the experiments were prepared with deionized water.

2.2. Instrument and software

Image capturing was performed using a Canon Lide 120 scanner (Canon Inc., Tokyo, Japan), and images were saved in JPEG format. The SPL microplates (The SPL Life Sciences, Pocheon, Korea) were used for sample placement within the scanner. To keep away from external light, all images were taken in a dark environment. Each sample was captured three times to ensure consistent image quality. The region of interest (ROI) was manually selected using the elliptical marquee tool in Adobe Photoshop CS5 2018 (Adobe Systems, Inc., San Jose, CA, USA) (Harris-

Love et al., 2016; Hua et al., 2020). The ROI selection focused on areas with distinguishable colors corresponding to the dyes, excluding background noise. This manual selection method, while direct and straightforward, may be subject to personal bias (Jia et al., 2020; Vidal & Amigo, 2012). To reduce this, all selections were reviewed by a trained individual, minimizing the potential impact of personal preferences. Adobe Photoshop provides various selection tools that facilitate the effective identification and isolation of the ROI for subsequent analysis (Wang et al., 2015).

Adobe Photoshop CS5 (2018) software was utilized to extract color channels from digital images. The extracted channels included Red (R), Green (G), and Blue (B) from the RGB model; Cyan (C), Magenta (M), Yellow (Y), and Black (K) from the CMYK model; grayscale (g); and Hue (H), Saturation (S), and Intensity (I) from the HSI model (Grudpan et al., 2015). MATLAB R2013a (The MathWorks, Natick, USA) software was applied to analyze the data, including color channels and color histograms. In order to convert digital image into histogram, free MATLAB “Imagens_gui” interface was used (Diniz, 2020). Color histograms were involving RGB, grayscale, and HSI. Average histograms were taken as input data to do calculations. Partial least squares regression (PLS) was done by MVC1_GUI toolbox in MATLAB (Amsaraj & Mutturi, 2024).

2.3. Univariate calibration method

Initially, digital images were captured for individual calibration solutions of Tar and SY. These images were converted into RGB and CMYK color models. The calibration curves were constructed by plotting each color channel against concentrations of Tar and SY. The best color channel was selected based on its linear relationship with the concentration of Tar and SY.

2.4. Multivariate calibration method

To simultaneously determine Tar and SY, color channels, effective color channels, and color histograms were applied as input data to construct PLS regression model.

The color channels including red, green, blue, cyan, magenta, yellow, black, grayscale and hue, saturation and intensity were evaluated and effective color channels were selected.

Effective color channels were identified based on their linear relationship with dye concentrations. Calibration plots were constructed for each color channel by plotting dye concentrations against the corresponding intensity values. Channels with the highest correlation coefficients ($R^2 \geq 0.99$) were selected as effective channels, ensuring the reliability and accuracy of these channels for quantifying dye concentrations in the samples. After determining the effective color channels, the contribution of the remaining color channels was evaluated using the forward feature selection method. Forward feature selection identifies the most significant attributes while eliminating irrelevant ones. In this approach, features are added one by one, and the model's accuracy is assessed at each step to see if it improves with the addition of the new feature. If accuracy does not increase or remains unchanged, those features are considered unnecessary and excluded. This process ensures that only essential features are retained in the final model. (Jia et al., 2020; Nakanishi et al., 2024; Rahma et al., 2023).

Additionally, PLS-assisted color histogram-based analytical systems was employed. Various color histogram combinations—such as Grayscale, RGB, HSI, Grayscale + RGB, Grayscale + HSI, RGB + HSI, and RGB + Grayscale + HSI—were assessed to build the regression model.

Twenty standard solutions were carefully prepared, containing a mixture of Tar and SY within linear ranges of 2–29 mg/L and 3–22 mg/L, respectively. Ten samples were randomly selected as calibration samples, while the remaining ten were used as prediction samples to evaluate the performance of the proposed method. The performance of the model in the calibration set was expressed by the coefficient of correlation for cross-validation (R_{CV}^2) and the root mean square error of cross-

Table 1

Figures of merit for determination of Tar and SY using scanner-based colorimetric method (yellow color channel) and HPLC.

Method	Analyte	Linear range (mg/L)	Equation	R ²	LOD ^(c) (mg/L)	LOQ ^(d) (mg/L)	RSD ^(e) (%)
Scanner-based colorimetry	Tar ^(a)	2–29	$Y = 7.3753 \times + 0.0146$	0.9998	0.6	2	0.6
	SY ^(b)	3–22	$Y = 9.5862 \times + 0.3693$	0.9988	0.9	3	1.2
HPLC	Tar	0.07–200	$Y = 28.67 \times + 16.408$	0.9995	0.02	0.07	2.0
	SY	0.07–200	$Y = 30.654 \times + 2.9899$	1	0.02	0.07	0.7

^a Tartrazine^b Sunset yellow^c Limit of detection^d Limit of quantitation^e Relative standard error.

validation (RMSECV). The model's predictive capability was assessed using the coefficient of determination for the prediction (R^2_{pred}), the root mean square error of prediction (RMSEP), and the relative error of prediction (REP). Additionally, the Elliptical Joint Confidence Region (EJCR) plot in the prediction model was considered to evaluate the model's accuracy and to check for any bias in the results (Fernandes et al., 2023; Qashqai & Heidari, 2023; Ramo et al., 2024).

2.5. Real sample analysis

One batch of 10 different commercially available non-alcoholic soft drink samples was collected from various markets in Iran. The selected drinks consisted of only one type: fruit-flavored, carbonated beverages. Ingredient labels indicated the presence of artificial colors, exclusively sunset yellow, though specific concentrations of this dye were not labeled.

The samples were degassed using an ultrasonic bath for 5 min. All samples, except for sample number 4, showed sunset yellow concentrations exceeding the linear range. To address this, these samples were diluted fivefold to bring their concentrations within acceptable levels. Sample number 4 was already within the linear range and did not require dilution. Deionized water was used as the solvent for the dilutions.

Subsequently, the initial concentrations of Tar and SY were simultaneously determined using the proposed method.

The performance of the proposed method was evaluated using a total of 10 independent replicates (10 samples) and 6 technical replicates.

2.6. Chromatographic analysis

The chromatographic analysis was performed using an Agilent 1100 HPLC system (Agilent Technologies, Santa Clara, CA, USA) equipped with a quaternary pump and a manual injection system with a 20 μ L injection loop. A Phenomenex C18 column of 4.6 \times 250 mm (Phenomenex Inc., Torrance, CA, USA) was utilized for the separation of the dyes. The mobile phase consisted of acetonitrile and methanol in a ratio of 80:20 (v/v), delivered at a flow rate of 1 mL/min. The analysis times were 5.6 min for Tar and 7.7 min for SY, with detection carried out at 445 nm using a UV detector. The column was maintained at room temperature throughout the analysis (Pedjie, 2012).

3. Result and discussion

3.1. Individual calibration of tartrazine and sunset yellow

The linearity of R, G, B, C, M, Y, K, and grayscale color channels was evaluated against the calibration concentrations of Tar and SY, individually. Among these, the yellow channel exhibited the strongest linear relationship with the concentrations. Table 1 compares the figures of merit for the scanner-based colorimetric method using the yellow channel with those obtained by the HPLC method for analysis of Tar and SY.

Table 2

Composition of calibration and prediction sets of Tar and SY for PLS regressions.

Number of samples	Calibration set		Prediction set	
	Tar ^(a) (mg/L)	SY ^(b) (mg/L)	Tar (mg/L)	SY (mg/L)
1	8.5	10	8	14
2	9.5	9.5	9	13
3	10.5	9	10	12.5
4	11	8.5	10.5	11.5
5	11.5	8.5	12	10
6	12	8	13	9
7	12.5	7.5	14	8
8	13	7	15	6.5
9	13.5	6.5	15.5	6
10	14	6	16	6

^a Tartrazine^b Sunset yellow.

3.2. Simultaneous determination of tartrazine and sunset yellow

The first stage in the simultaneous determination of the binary mixture of Tar and SY with the multivariate calibration method involved the construction of the calibration and prediction sets. The composition of the calibration and prediction sets is provided in Table 2. These sets were designed to include a representative range of concentrations to ensure the robustness of the calibration models and the reliability of the predictions. The randomization of sample selection helped to minimize potential systematic errors and validated the applicability of the method across different concentrations.

In this study, Tar and SY were simultaneously determined using the PLS regression method, a robust chemometrics technique that facilitates the analysis of multiple variables simultaneously (Wold et al., 2001). Various input data, including color channels, effective color channels, and color histograms were evaluated.

3.2.1. PLS-assisted color channels -based analytical systems

The analysis involved a comprehensive evaluation of the color channels, including red, green, blue (RGB), cyan, magenta, yellow, black (CMYK), grayscale, as well as hue, saturation, and intensity (HSI) for constructing PLS regression method. The results are summarized in Table 3.

The R^2_{pred} were found to be 0.9913 for Tar and 0.9931 for SY, indicating a strong predictive capability of the multivariate calibration model.

In Fig. 1(a, c), predicted values are plotted against actual values for both dyes. The random scatter of points around the line suggests that the model's predictions are free from systematic error and are unbiased, which confirms the reliability of the calibration method.

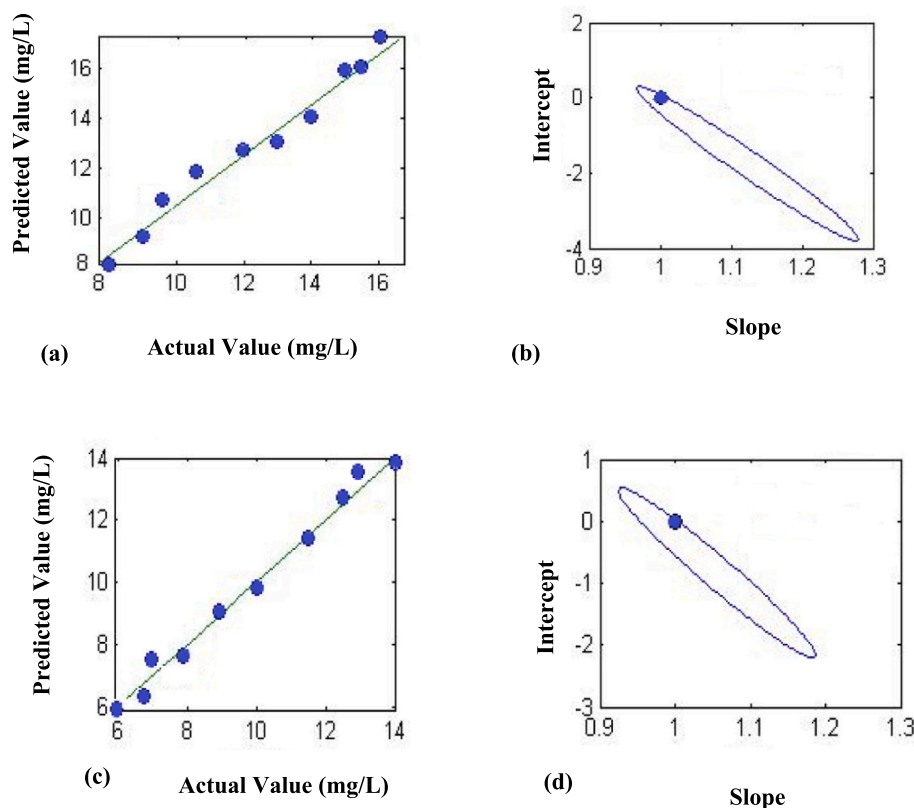
The EJCR region forms an elliptical shape, and it examines whether the theoretically expected values (slope = 1 and intercept = 0) fall within this ellipse. When the ideal point is included in the EJCR, it confirms the accuracy of the methodology (Lozano et al., 2014). Fig. 1(b, d) illustrates the EJCR plots (at 95 % confidence level) for analysis of Tar

Table 3

Results of PLS-assisted color channels for simultaneous determination of Tar and SY.

Color channels	Analyte	Calibration			Prediction		
		LV ^(c)	R _{CV} ^(d)	RMSECV ^(e) (mg/L)	R _{Pred} ^(f)	RMSEP ^(g) (mg/L)	REP ^(h) (%)
RGB+ CMYK+ grayscale+ HSI	Tar ^(a)	3	0.2349	0.31	0.9913	0.54	4.3
	SY ^(b)	3	0.3833	0.30	0.9931	0.43	4.4

R: Red; G: Green; B: Blue; C: Cyan; M: Magenta; Y: Yellow; K: Black; g: grayscale; H: Hue; S: Saturation; I: Intensity.

^a Tartrazine^b Sunset yellow^c Latent variable^d Coefficient of determination for cross-validation^e Root mean square error of cross validation^f Coefficient of determination for the prediction^g Root mean square error of prediction^h Relative error of prediction.**Fig. 1.** PLS results and EJCR plots of predicted vs. actual values using the color channels for Tar (a, b) and SY (c, d).

and SY. As seen, they reveal the absence of bias.

The study highlights the potential of digital scanner images as a practical tool for simultaneous determination of the dyes in mixture samples (Botelho et al., 2014).

3.2.2. PLS-assisted effective color channels -based analytical systems

In this study, feature selection was applied to identify effective color channels to simplify PLS regression and enhance the model's performance (Canero et al., 2024; Lin et al., 2023). As described in Section 2.4, effective color channels were identified based on the linear relationship between dye concentrations and each color channel using univariate calibration for Tar and SY individually ($R^2 \geq 0.99$). The results indicated that the Green, Blue, Yellow, grayscale, Saturation, and Intensity were the most effective color channels for determining both Tar and SY (Table 4). This targeted approach led to a significant improvement in the R_{CV}^2 , which increased to 0.8468 for Tar and 0.8759 for SY. As a result, the RMSECV decreased to 0.14 mg/L for Tar and 0.23 mg/L for SY,

highlighting the effectiveness of the model. Additionally, after determining the effective color channels, the contribution of the remaining color channels was evaluated using the forward feature selection method (Table 4). No significant improvement in the performance of PLS for the simultaneous analysis of Tar and SY was observed. As a result, the Green, Blue, Yellow, grayscale, Saturation, and Intensity were considered as the optimal channels for simultaneous determination of Tar and SY in mixture samples using PLS regression.

These enhancements in model performance highlight the critical importance of feature selection in multivariate calibration. Previous studies have similarly demonstrated that selecting relevant features can substantially improve the robustness and predictive accuracy of PLS regression (Amsaraj & Mutturi, 2021 & Amsaraj & Mutturi, 2023).

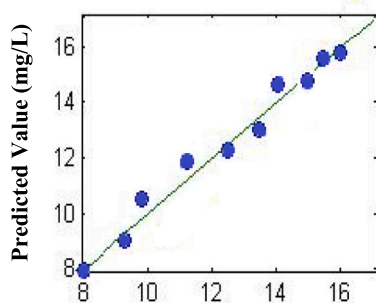
Fig. 2 illustrates the predicted concentrations of Tar and SY against the actual values. The EJCR plots indicate that reliable results were achieved.

Table 4

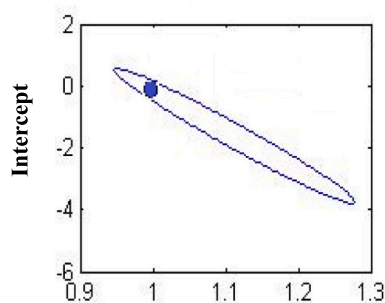
Results of PLS-assisted effective color channels for simultaneous determination of Tar and SY.

Selected Color Channels	Analyte	Calibration			Prediction		
		LV ^(c)	R _{CV} ^(d)	RMSECV ^(e) (mg/L)	R ² _{Pred} ^(f)	RMSEP ^(g) (mg/L)	REP ^(h) (%)
GBYgSI	Tar ^(a)	6	0.8468	0.14	0.9938	0.48	3.9
	SY ^(b)	5	0.8759	0.23	0.9968	0.23	2.4
GBYgSI+ R	Tar	4	0.2190	0.24	0.9922	0.54	4.4
	SY	4	0.2426	0.23	0.9949	0.29	2.9
GBYgSI+C	Tar	5	0.1300	0.29	0.9903	0.58	4.6
	SY	3	0.6690	1.09	0.9921	0.37	3.8
GBYgSI+M	Tar	3	0.3434	0.44	0.9886	0.82	6.6
	SY	3	0.1237	0.42	0.9900	0.92	9.4
GBYgSI+K	Tar	5	0.7609	0.29	0.9931	0.56	4.5
	SY	5	0.1221	0.31	0.9917	0.24	2.4
GBYgSI+H	Tar	4	0.5415	0.32	0.9914	0.53	4.3
	SY	4	0.2200	0.21	0.9944	0.30	3.1

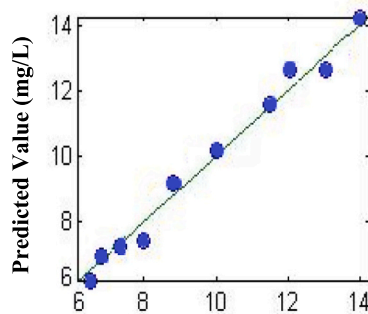
*R: Red; G: Green; B: Blue; C: Cyan; M: Magenta; Y: Yellow; K: Black; g: grayscale; H: Hue; S: Saturation; I: Intensity.

^a Tartrazine^b Sunset yellow^c Latent variable^d Coefficient of determination for cross-validation^e Root mean square error of cross validation^f Coefficient of determination for the prediction^g Root mean square error of prediction^h Relative error of prediction.

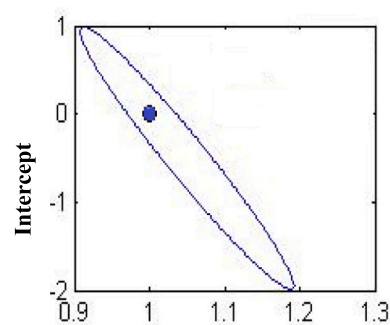
(a) Actual Value (mg/L)



(b) Slope



(c) Actual Value (mg/L)



(d) Slope

Fig. 2. PLS results and EJCR plots of predicted vs. actual values using effective color channels for Tar (a, b) and SY (c, d).

3.2.3. PLS-assisted color histogram-based analytical systems

In image processing, a color histogram is a quantitative representation of the distribution of color intensities in a digital image (Swain & Ballard, 1991; Zhang et al., 1995).

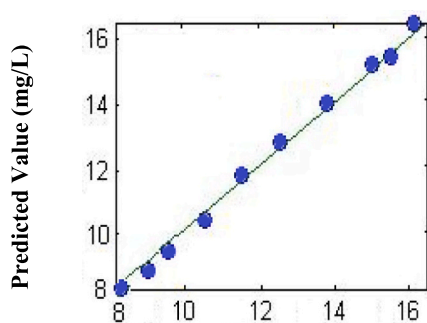
The color histogram can be built for any kind of color model including RGB, HSI, HSV and gray scale. Pre-processing techniques, such as noise reduction and image segmentation based on pixels or edges,

may be applied to the color channels to enhance the quality of the data (Diniz, 2020). However, one of the major advantages of using color histograms is their simplicity; they allow for quick and direct extraction of information without the need for complex pre-processing, enabling data to be analyzed in its original form (De Sousa Fernandes et al., 2019; Reile et al., 2020). The use of color histograms as an analytical signal emerges as a good alternative, because they provide a straightforward

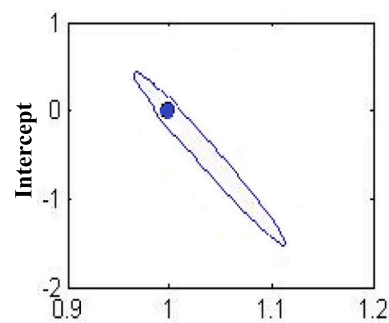
Table 5

Results of PLS-assisted color histogram for simultaneous determination Tar and SY.

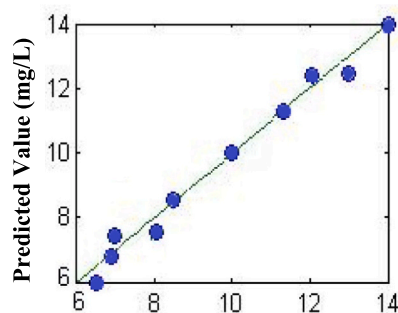
Color histogram	Analyte	Calibration			Prediction		
		LV ^(c)	R _{CV} ² ^(d)	RMSECV ^(e) (mg/L)	R ² _{Pred} ^(f)	RMSEP ^(g) (mg/L)	REP ^(h) (%)
Grayscale	Tar ^(a)	3	0.8643	1.32	0.8928	1.40	11.2
	SY ^(b)	3	0.8865	1.23	0.9232	1.01	10.4
RGB	Tar	4	0.8812	0.89	0.9229	1.20	9.9
	SY	4	0.9092	0.91	0.9477	1.22	12.5
HSI	Tar	3	0.8901	0.64	0.9377	0.93	7.5
	SY	5	0.9298	0.71	0.9622	1.04	10.7
Grayscale+RGB	Tar	3	0.8955	0.84	0.9346	1.10	9.05
	SY	4	0.9100	2.15	0.9592	1.20	11.9
Grayscale+HSI	Tar	4	0.9023	0.53	0.9469	0.87	6.9
	SY	5	0.9211	1.54	0.9680	1.00	10.3
RGB + HSI	Tar	4	0.9078	0.53	0.9422	0.91	7.2
	SY	5	0.9261	0.36	0.9667	1.00	10.3
RGB + Grayscale+ HSI	Tar	6	0.9572	0.10	0.9977	0.21	1.6
	SY	6	0.9519	0.13	0.9989	0.10	1.0

^a Tartrazine^b Sunset yellow^c Latent variable^d Coefficient of determination for cross-validation^e Root mean square error of cross validation^f Coefficient of determination for the prediction^g Root mean square error of prediction^h Relative error of prediction.

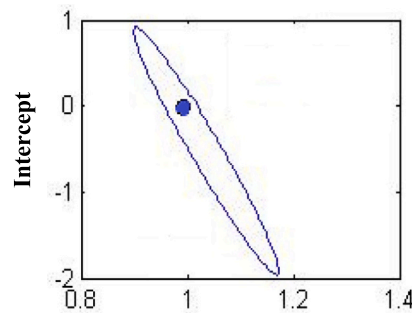
(a) Actual Value (mg/L)



(b) Slope



(c) Actual Value (mg/L)



(d) Slope

Fig. 3. PLS results and EJCR plot of predicted vs. actual values using RGB + Grayscale + HSI histograms for Tar (a, b) and SY (c, d).

method for rapid acquisition of the analytical information when coupled with multivariate chemometrics methods (Diniz, 2020; De Moraes & de Lima, 2015).

Although color histogram analysis provides valuable insights into the

distribution of color intensities, interpreting the results can be challenging due to the inherent complexity of frequency distributions (Diniz, 2020; Reile et al., 2020).

In this study, color histograms were generated for Grayscale, RGB,

Table 6

Quantification results of optimal models for simultaneous determination of Tar and SY using PLS-assisted color channels, effective color channels, and color histograms.

Input data	Analyte	Calibration			Prediction		
		LV ^(c)	R _{CV} ^(d)	RMSECV ^(e) (mg/L)	R _{Pred} ^(f)	RMSEP ^(g) (mg/L)	REP ^(h) (%)
Color channels	Tar ^(a)	3	0.2349	0.31	0.9913	0.54	4.3
	SY ^(b)	3	0.3833	0.30	0.9931	0.43	4.4
Effective color channels	Tar	6	0.8468	0.14	0.9938	0.48	3.9
	SY	5	0.8759	0.23	0.9968	0.23	2.4
Color histograms	Tar	6	0.9572	0.10	0.9977	0.21	1.6
	SY	6	0.9519	0.13	0.9989	0.10	1.0

*R: Red; G: Green; B: Blue; C: Cyan; M: Magenta; Y: Yellow; K: Black; g: grayscale; H: Hue; S: Saturation; I: Intensity.

^a Tartrazine

^b Sunset yellow

^c Latent variable

^d Coefficient of determination for cross-validation

^e Root mean square error of cross validation

^f Coefficient of determination for the prediction

^g Root mean square error of prediction

^h Relative error of prediction.

Table 7

Simultaneous determination of Tar and SY in soft drinks using PLS-assisted RGB+ Grayscale+ HSI histograms and HPLC.

Sample	PLS-assisted RGB+ Grayscale+ HSI histograms				HPLC				
	Tar ^(a)		SY ^(b)		Tar		SY		
	Con. (mg/L)	RSD (%)	Con. (mg/L)	RSD (%)	Con. (mg/L)	RSD (%)	Con. (mg/L)	RSD (%)	t-value ^(g)
S1	ND ^(c)	—	30.0 ^(d) ± 0.5 ^(e)	1.6	ND	—	30.37 ^(f) ± 2.1	4.6	0.51
S2	ND	—	33.1 ± 0.9	2.6	0.28 ± 0.01	2.7	33.9 ± 0.4	0.7	1.14
S3	ND	—	21.2 ± 0.3	1.3	0.18 ± 0.01	4.7	21.2 ± 0.7	2.2	0.69
S4	ND	—	12.1 ± 0.2	2.0	ND	—	12.8 ± 0.6	2.7	1.51
S5	ND	—	27.6 ± 0.8	1.7	0.13 ± 0.02	2.8	27.4 ± 0.4	0.8	0.67
S6	ND	—	48.2 ± 0.6	1.2	ND	—	48.39 ± 2.2	2.9	0.27
S7	ND	—	40.2 ± 0.8	1.8	0.191 ± 0.006	2.0	40.5 ± 0.7	1.2	0.49
S8	ND	—	50.8 ± 1.1	2.1	0.166 ± 0.003	4.0	50.96 ± 1.4	1.7	0.26
S9	ND	—	48.5 ± 0.6	1.3	ND	—	48.6 ± 0.6	1.3	0.26
S10	ND	—	45.2 ± 1.0	2.1	ND	—	45.4 ± 0.5	0.7	0.20

^a Tartrazine

^b Sunset yellow

^c Not detected

^d Mean of 6 replicates of measurement

^e Confidence Interval ($\alpha = 0.05, N = 6$)

^f Mean of 3 replicates of measurement

^g For seven degrees of freedom at 95 % confidence level, the tabulated t-value is 2.36.

HSI, Grayscale + RGB, Grayscale + HSI, RGB + HSI, and RGB + Grayscale + HSI color models to build the PLS model for the simultaneous determination of Tar and SY.

The results, presented in Table 5, indicate that combination of RGB + Grayscale + HSI color histograms provided the best predictive performance. The RMSECV values were recorded at 0.10 mg/L for Tar and 0.13 mg/L for SY. The R_{Pred}² values were exceptionally high at 0.9977 and 0.9989 for Tar and SY, respectively.

As shown in Table 5, data combination has enhanced the performance of the multivariate calibration model, underscoring its strong predictive capability (Fig. 3). The improved results due to this solution, color histogram combination, were demonstrated in several studies De Sousa Fernandes et al., 2019; Reile et al., 2020).

The results in Table 6 clearly demonstrate that all PLS models incorporating the color channels (RGB, CMYK, grayscale, HSI), effective color channels (Green, Blue, Yellow, grayscale, Saturation, Intensity), and color histogram combination (RGB+ Grayscale+ HSI) were suitable for simultaneous prediction of Tar and SY, achieving REP values lower

than 5 % and R_{Pred}² values higher than 0.99. As shown, the PLS-assisted RGB+ Grayscale+ HSI histograms achieved the best overall predictive performance (Table 6). From a food analysis perspective, it is essential to develop new methods that ensure both high accuracy and precision. In this study, the PLS-assisted RGB+ Grayscale+ HSI histograms were therefore applied for the quantification of Tar and SY in soft drink samples.

3.3. Real sample analysis

To signify the applicability of the PLS-assisted RGB+ Grayscale + HSI histograms, the simultaneous determination of Tar and SY in 10 soft drink samples was performed and compared with HPLC (Table 7). These real samples were not spiked with analytes, and the concentrations of Tar in the soft drinks were below the LOD determined by scanner-based colorimetry. As a result, Tar could not be detected. The relative standard deviation (RSD) values for six replicate measurements were ≤ 2.6 % using the PLS-assisted RGB+ Grayscale+ HSI histograms-based method

Table 8

Simultaneous determination of Tar and SY in a spiked soft drink sample (sample: S1) by PLS-assisted RGB+ Grayscale+ HSI histograms and HPLC.

Added (mg/L)	Found (mg/L)		Recovery (%) ^(b)		RSD (%)		t-test ^(g)
	PLS	HPLC	PLS	HPLC	PLS	HPLC	
0	ND ^(c)	ND	—	—	1.5	2.7	—
30	30.5 ^(d) ± 0.5 ^(e)	30.4 ^(f) ± 0.9	101.6	101.5	2.1	2.5	0.04
35	35.5 ± 0.7	35.3 ± 1.0	101.4	100.8	1.4	2.4	0.41
40	39.9 ± 0.6	40.4 ± 1.1	99.7	101.1	1.5	2.7	1.17
SY ^(h)							
0	30.3 ± 0.6	30.3 ± 1.1	—	—	2.0	3.7	0.06
20	50.3 ± 1.4	50.6 ± 1.2	99.8	101.6	2.7	2.4	0.49
25	55.6 ± 0.8	55.2 ± 1.9	101.3	99.3	1.4	3.5	0.22
30	60.7 ± 1.3	60.1 ± 1.9	101.3	99.0	2.1	3.2	0.6

^a Tartrazine

^b Recovery (%) = $\frac{C_{\text{found}} - C_{\text{real}}}{C_{\text{added}}} \times 100$

^c Not detected

^d Mean of 6 replicates of measurement

^e Confidence Interval ($\alpha = 0.05$, $N = 6$)

^f Mean of 3 replicates of measurement;

^g For Nine degrees of freedom at 95 % confidence level, the tabulated t-value is 2.26

^h Sunset yellow.

and were not ≥ 4.6 % for three replicate determinations using the HPLC method.

To validate the accuracy of Tar and SY determination in the soft drink samples, a *t*-test was conducted to compare the results obtained using PLS-assisted RGB + Grayscale + HSI histograms and HPLC. The calculated *t*-value is presented in Table 7. At the 95 % confidence level, the difference between the results obtained by the two methods was not statistically significant, as the *t*-value was lower than the critical *t*-value (Abdelwahed et al., 2024). In summary, it can be concluded that the two methods produce comparable results.

To ensure a more robust evaluation of the proposed method's performance, in addition to the analysis of real samples, Tar and SY were simultaneously determined in a spiked sample (S1) containing known concentrations. To validate the obtained results, Tar and SY in the spiked sample were also analyzed using HPLC, and the recovery results are summarized in Table 8.

The recoveries achieved using the PLS-assisted RGB+ Grayscale+ HSI histograms ranged from 99.7 % to 101.6 %, with a mean recovery of 100.9 % for Tar. For SY, recoveries ranged from 99.9 % to 101.3 %, with a mean recovery of 100.8 %. The HPLC method also demonstrated strong performance, yielding mean recoveries of 101.4 % for Tar and 100.3 % for SY.

To sum up the findings, the satisfactory results obtained using the PLS-assisted RGB+ Grayscale + HSI histograms indicate that this method provides results comparable to those of HPLC. The *t*-test indicates that the results obtained from the developed and standard methods are equivalent (Table 8).

These findings further highlight the proposed method's potential for routine analysis in the beverage industry, demonstrating its reliability for quality control purposes.

The analytical parameters of PLS-assisted RGB + Grayscale+ HSI histograms and several other methods for the determination of Tar and SY were compared in Table 9. The results indicate that this method

Table 9

Comparison of this study with the literature.

Analyte	Real sample	Digital device	Color model	Multivariate calibration method	Linear range (mg/L)	R ²	LOD ^(c) (mg/L)	RMSECV ^(d) (mg/L)	RMSEP ^(e) (mg/L)	REP ^(f) (%)	Ref.
SY ^(a)	Orange beverages	Scanner	RGB	PLS	7.8–39.7	0.9702	NR ^(g)	1.3	1.3	NR	Botelho et al., 2014
SY	Chocolate-orange, Jelly-yellow	Smartphone	RGB	NR	25–500	0.9981	5.28	NR	NR	NR	Saadati, 2021
SY	Chocolated orange, Soft drink orange, Jelly powdered watermelon	Scanner	RGB	NR	30–250	0.9989	7.70	NR	NR	NR	Sorouraddin et al., 2015
Tar ^(b)	Soda drinks	Smartphone	RGB HSV	PLS	0–20	0.9953	1.2	NR	NR	NR	Jacinto et al., 2023
Tar	Ice-pop, Liquid candy, Liquid sweetener, Liqueur beverage, Food Coloring	Scanner	RGB	PLS	6–40	NR	1.8	3.3	3	NR	Vidal et al., 2018
SY	Soft drinks	Scanner	RGB+ Grayscale + HSI histograms	PLS	2–29	0.9988	0.9	0.13	0.10	1.6	This study
Tar	Soft drinks	Scanner	RGB+ Grayscale + HSI histograms	PLS	3–22	0.9998	0.6	0.10	0.21	1.0	This study

^a Sunset yellow

^b Tartrazine

^c Limit of detection

^d Root mean square error of cross validation

^e Root mean square of error prediction

^f Relative error of prediction

^g Not reported.

offers significantly better applicability for accurate and precise simultaneous analysis of these analytes in real samples.

4. Conclusion

In this study, digital images captured using a flatbed scanner were transformed into various color models, including RGB, CMYK, and HSI, to serve as multivariate input data for PLS models. The flatbed scanner, an inexpensive and widely accessible tool in most laboratories, offers the advantages of fast image acquisition and user-friendly processing. A significant limitation of colorimetric methods is the lack of specificity validation. Specificity refers to the method's ability to discriminate between the desired analytes and interferences present in real samples. To resolve this limitation, in addition to the analysis of real samples, Tar and SY were simultaneously determined in a spiked sample containing known concentrations of the analytes. The results indicated that PLS models utilizing color channels (RGB, CMYK, grayscale, HSI), effective color channels (Green, Blue, Yellow, Saturation, Intensity), and combined color histograms (RGB + Grayscale + HSI) were suitable for predicting Tar and SY simultaneously. Among these, the PLS-assisted RGB + Grayscale + HSI histograms provided the best overall predictive performance. Satisfactory results were achieved in analyzing Tar and SY in soft drink samples using this approach, yielding outcomes comparable to those obtained with HPLC. However, unlike HPLC, which is time-consuming, costly, and requires solvents and skilled personnel, the proposed method is cost-effective, rapid, and easy to operate and implement. These attributes highlight its potential as a practical alternative for routine analysis of synthetic dyes in beverages.

CRediT authorship contribution statement

Seyyede Fatemeh Hosseini: Writing – original draft, Methodology, Formal analysis, Data curation. **Tahereh Heidari:** Supervision. **Ameneh Zendegi-Shiraz:** Validation. **Majid Ameri:** Validation.

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.

Data availability

Data will be made available on request.

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