

Article

VIS/NIR Spectroscopy as a Non-Destructive Method for Evaluation of Quality Parameters of Three Bell Pepper Varieties Based on Soft Computing Methods

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Abstract: Spectroscopic analysis was employed to evaluate the quality of three bell pepper varieties within the 350–1150 nm wavelength range. Quality parameters such as firmness, pH, soluble solids content, titratable acids, vitamin C, total phenols, and anthocyanins were measured. To enhance data reliability, principal component analysis (PCA) was used to identify and remove outliers. Raw spectral data were initially modeled using partial least squares regression (PLSR). To optimize wavelength selection, support vector machines (SVMs) were combined with genetic algorithms (GAs), particle swarm optimization (PSO), ant colony optimization (ACO), and imperial competitive algorithm (ICA). The most effective wavelength selection method was subsequently used for further analysis. Three modeling techniques—PLSR, multiple linear regression (MLR), and artificial neural networks (ANNs)—were applied to the selected wavelengths. PLSR analysis of raw data yielded a maximum R^2 value of 0.98 for red pepper pH, while the lowest R^2 (0.58) was observed for total phenols in yellow peppers. SVM-PSO was determined to be the optimal wavelength selection algorithm based on ratio of performance to deviation (RPD), root mean square error (RMSE), and correlation values. An average of 15 effective wavelengths were identified using this combined approach. Model performance was evaluated using root mean square error of cross-validation and coefficient of determination (R^2). ANN consistently outperformed MLR and PLSR in predicting firmness, pH, soluble solids content, titratable acids, vitamin C, total phenols, and anthocyanins for all three varieties. R^2 values for the ANN model ranged from 0.94 to 1.00, demonstrating its superior predictive capability. Based on these results, ANN is recommended as the most suitable method for evaluating the quality parameters of bell peppers using spectroscopic data.

Keywords: non-destructive evaluation; spectroscopy; bell pepper; quality parameter



Citation: Latifi Amoghin, M.; Abbaspour-Gilandeh, Y.; Tahmasebi, M.; Kaveh, M.; El-Mesery, H.S.; Szymanek, M.; Sprawka, M. VIS/NIR Spectroscopy as a Non-Destructive Method for Evaluation of Quality Parameters of Three Bell Pepper Varieties Based on Soft Computing Methods. *Appl. Sci.* **2024**, *14*, 10855. <https://doi.org/10.3390/app142310855>

Academic Editor: Alessandra Biancolillo

Received: 22 October 2024

Revised: 16 November 2024

Accepted: 19 November 2024

Published: 23 November 2024



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1. Introduction

Bell pepper (*Capsicum annuum* L.) is a commercially valuable crop widely cultivated for its desirable flavor. Rich in essential vitamins (A, B, C, and E) and various antioxidant phytochemicals [1], it has become a dietary staple worldwide. The global production of bell pepper reached an impressive 793,000 tons in 2021 [2], driving the demand for efficient production and high-quality sorting methods. Bell pepper quality is a complex trait influenced by factors such as color, firmness, soluble solids, dry matter, and vitamin C content [3–5]. Its nutritional value has contributed to its prominent position in global diets [4].

Prolonged fruit retention in the parent plant can induce significant physiological changes, affecting aging and nutritional composition, including total soluble solids, ascorbic acid, pH, and titratable acidity [6]. Bell pepper respiration persists post-harvest, as ripening continues [7]. Consequently, carotenoid levels increase while chlorophyll content declines, accompanied by alterations in internal composition [8,9]. Therefore, accurate assessment of harvested product quality is crucial for effective distribution and marketing. While mechanical and manual sorting often relies on appearance, it overlooks critical internal quality attributes.

Advanced non-destructive methods are increasingly employed for evaluating, grading, and sorting fruits and vegetables. These techniques, encompassing optical (image processing, spectroscopy, hyperspectral imaging, thermal imaging), mechanical (acoustic-ultrasound, vibration, and impact sound analysis), electromagnetic, X-ray (X-ray CT), dielectric, and electronic nose technologies, have shown promise in enhancing post-harvest quality and market value. Agricultural engineering has successfully leveraged advanced sensors and machine vision to overcome the limitations of traditional destructive testing methods, reducing labor costs and human error in the classification process [4].

Machine vision and spectroscopy have emerged as promising non-destructive techniques for quality control in agricultural science. These technologies find applications across diverse fields including terrestrial and aerial mapping, agricultural product monitoring, precision agriculture, robotics, autonomous navigation, product evaluation, quality assurance, and prediction of physiochemical properties [10]. Extensive research has been conducted on employing machine vision to classify bell peppers based on maturity level and size [11], measure color parameters [12], and estimate overall maturity [13].

Near-infrared (NIR) spectroscopy is a versatile analytical technique with applications spanning medicine, agriculture, chemistry, and other fields. This environmentally friendly method offers a cost-effective alternative to traditional approaches, often eliminating the need for sample preparation [14]. In the realm of fruit analysis, NIR spectroscopy provides valuable spectral data that can be used to assess physiochemical properties and detect defects [15].

Recent studies have demonstrated the potential of non-destructive techniques for evaluating various quality parameters in fruits and vegetables. NIR spectroscopy has been successfully applied to predict total soluble solids in strawberries [16]. Drying methods have been investigated for their impact on apple, plum, and their mixtures [17]. Chlorophyll fluorescence measurements have enabled the determination of ripening stages and sorting of bell pepper fruit [18]. Other studies have focused on non-destructive prediction of internal apple characteristics such as texture, acidity, and starch content [19], peach variety detection [20], eggplant chilling injury assessment [21], measurement of quality parameters of apple fruit [22], quality measurement for three varieties of tomato [23]. Research has also explored the quality characteristics of sweet red pepper paste [24], the ripening stages of lamuyo pepper [25], capsaicin content and pepper powder adulteration [26], antioxidant activity and water content in chili powder (*Capsicum annuum* L.) [27], vitamin C and antioxidant activity of intact red chilies [28], quality compounds in *Capsicum* species (*Capsicum annuum* L. and *Capsicum frutescens* L.) [29], chili powder antioxidant activity classification (*Capsicum annuum* L.) [30], total carotene and vitamin C determination in red pepper powder [31], and the impact of skin thickness on soluble solids content in fruits [32]. Therefore, according to the research conducted in this field, it can be seen that non-destructive techniques have the ability to improve the evaluation and control of the quality of fruits and vegetables.

The VIS/NIR spectroscopy, as a non-destructive method, has been applied in assessing the quality of various agricultural products, offering advantages such as high speed and accuracy. However, focus on the evaluation of different varieties of bell pepper and the specific quality attributes considered in this study has received less attention from researchers. This study addresses this gap by exploring the use of VIS/NIR spectroscopy for a rapid and accurate assessment of bell pepper quality. The findings of this research

could contribute to the improvement and standardization of quality assessments for this product within the agricultural supply chain and processing industries. Therefore, the aim of this study is to investigate the feasibility of using visible/near-infrared (VIS/NIR) spectroscopy as a rapid and non-destructive method for determining the quality parameters of bell peppers. Given the importance of accurately assessing the quality of agricultural products and the need for a method that is both time-efficient and non-invasive, this study seeks to achieve this goal by developing a partial least squares (PLS) model. In this regard, the wavelengths influencing bell pepper quality were identified using soft computational techniques, and multiple modeling approaches were employed for more precise analysis. Ultimately, this research aims to offer an optimized method capable of performing quality assessments of this product with high accuracy and speed for use in the agricultural and packaging industries.

2. Materials and Methods

2.1. Raw Materials and Chemicals

Three bell pepper varieties—red (Pasarella RZ F1), yellow (Kaliroy RZ F1), and orange (Bachata RZ F1)—were procured from local greenhouses. From each variety, 30 uniformly sized, shaped, and colored fruits were selected, ensuring no signs of mechanical damage or fungal infection. To equilibrate with the laboratory temperature, samples were maintained at 25 °C for 2 h prior to analysis. For destructive analyses, phenolphthalein, potassium iodate (KIO₃), hydrochloric acid (HCl), potassium iodide (KI), ethanol, and Folin–Ciocalteu reagent were procured from Merck (Darmstadt, Germany). Sodium hydroxide (NaOH), methanol, hydrochloric acid, and sodium carbonate were supplied by Mojallali (Tehran, Iran), while starch was generously provided by Glucosan (Tehran, Iran).

2.2. Vis/NIR Spectroscopy

Vis/NIR spectroscopy was performed using a PS-100 model spectrometer (Apogee Instruments, Inc., Logan, UT, USA). Equipped with a CCD detector, the spectrometer offered a resolution of 1 nm across a spectral range of 350–1150 nm. A halogen–tungsten light source was employed. Spectra were acquired via a USB connection to a computer and processed using Spectra Wiz software V6.32. Prior to sample analysis, dark and white reference spectra were established. The dark spectrum was recorded with the light source off, while a standard Teflon disk served as the white reference under illumination. Spectral data were collected from four distinct points on each sample. These individual spectra were averaged to generate an absorption spectrum for each sample [22]. Ultimately, 90 spectral data points were extracted for subsequent analysis.

2.3. Qualitative Property Tests (Destructive)

2.3.1. Firmness

Fruit firmness was determined using a stainless-steel rod (6 mm diameter) connected to a fruit firmness test device (STEP SYSTEM, Nürnberg, Germany; detection limit 0.05–196.10 N). The maximum penetration force was recorded as the firmness index. Measurements were taken at three equidistant points on the fruit's central periphery [33].

2.3.2. Soluble Solid Content (SSC)

Soluble solid content (SSC) was determined using a digital refractometer (PrismaT-ech BPTR50, Karaj, Iran). The instrument has a detection range of 0–100% Brix with an accuracy of ± 0.05 Brix. A drop of juice was applied to the refractometer's glass prism for measurement.

2.3.3. pH

The pH of the fruit juice was determined using a Metrohm 827 digital pH meter (Zofingen, Switzerland) at ambient temperature. This instrument has a detection range of 1–14 pH and an accuracy of ± 0.003 pH. The juice was transferred to a Falcon tube for pH measurement, which was obtained by immersing the electrode directly into the sample [34].

2.3.4. Titratable Acidity (TA)

Titrateable acidity (TA) was determined by titration with 0.1 mol/L sodium hydroxide (NaOH) solution. Phenolphthalein was used as an indicator, and the titration was continued until a stable light pink color was reached, corresponding to a pH of approximately 8. For this analysis, 5 mL of fruit juice was mixed with 1 mL of phenolphthalein solution (10 g/m) and diluted to a total volume of 200 mL with distilled water. The titration endpoint was indicated by a persistent light pink color of the diluted extract. The calculated TA was expressed in terms of malic acid (the predominant fruit acid) according to Equation (1).

$$TA = \frac{mL(NaOH) \times N(NaOH) \times \text{acidmeq.factor}}{mL(\text{juice})} \times 100 \quad (1)$$

TA represents the percentage of titrateable acidity. mL(NaOH) is the volume of sodium hydroxide (NaOH) consumed during titration. N(NaOH) denotes the normality of the consumed NaOH, which is 0.1 mol/L. The acidmeq factor is the acid equivalent factor of the dominant fruit acid, equaling 0.067. Finally, mL(juice) signifies the fruit juice volume, which is 5 mL [35].

2.3.5. Ascorbic Acid

Ascorbic acid content was determined using a titration method with potassium iodate (KIO_3) as the titrant and starch solution (5% *w/v*) as the indicator. A 20 mL aliquot of fruit juice was diluted to 150 mL with distilled water. Subsequently, 1 mL of starch solution, 5 mL of 1 M hydrochloric acid (HCl), and 5 mL of 0.006 M potassium iodide (KI) were added. The solution was then titrated with 0.002 M potassium iodate until a persistent blue color appeared, indicating the endpoint. The ascorbic acid content was calculated using Equation (2).

$$\text{Vit C} = \frac{5.2836 V}{10^3} \quad (2)$$

In the equation above, Vit C represents the ascorbic acid (vitamin C) content expressed as milligrams per 100 mL of juice, while V denotes the consumed iodate volume in μL [36].

2.3.6. Anthocyanin

Anthocyanin content was determined using the Fuleki and Francis method (1968) [37]. Fruit peel (100 mg) was ground in 10 mL of acidic methanol (99% methanol, 1% hydrochloric acid). The homogenate was transferred to Falcon tubes and centrifuged at 6000 rpm for 10 min at 4 °C (LISA 2.5L centrifuge AFI, Château-Gontier, France). The supernatant was stored in darkness at room temperature for 24 h. Anthocyanin absorbance was measured at 550 nm and 25 °C using a NanoDrop One C spectrophotometer (Thermo Scientific, Waltham, MA, USA; detection limit 0.06–820 mg/mL). Anthocyanin concentration was calculated according to Equation (3).

$$C = 528.89 \times 10^3 \frac{A}{\epsilon b} \quad (3)$$

where C represents the anthocyanin content (mg/g), A is the absorbance measured at 550 nm, ϵ denotes the extinction coefficient, and b is the path length (width) of the cuvette.

2.3.7. Total Phenol

Total phenol content was determined using a modified Folin–Ciocalteu method [38]. Briefly, one gram of sample tissue was homogenized in an ice bath using a porcelain mortar with 10 mL of 80% ethanol. The homogenate was transferred to Falcon tubes and centrifuged at 4 °C, 4000 rpm for 10 min (LISA 2.5L centrifuge AFI, France). The supernatant was subjected to phenol analysis. For the phenol assay, 30 µL of supernatant was mixed with 600 µL of 10% (*v/v*) Folin–Ciocalteu reagent and 90 µL of distilled water. After 6 min, 480 µL of 7% (*w/v*) sodium carbonate solution was added. A water-based blank was prepared similarly. Absorbance was measured at 765 nm and 25 °C using a NanoDrop™ OneC spectrophotometer (Thermo Fisher Scientific, Waltham, MA, USA). Total phenol content was calculated from a standard curve generated using gallic acid (mg/g sample).

2.4. Data Analysis

2.4.1. Principal Component Analysis (PCA) and Outlier Detection

Various factors, including technical issues, data collection errors, and incorrect sampling, can lead to the formation of improper samples, or outliers, during testing. To address this, principal component analysis (PCA) was initially employed to reduce data dimensionality. Subsequently, Hotelling's T^2 test was applied to identify outliers within the PCA-derived multidimensional space.

2.4.2. Partial Least Squares Regression (PLSR) and Finding Effective Wavelengths

Non-destructive methods based on full-range spectroscopy are impractical due to their high cost and time consumption. Consequently, identifying and minimizing the effective wavelength range is essential. This study initially applied a partial least squares regression (PLSR) model to the complete dataset. To evaluate the model's performance, data were randomly partitioned into calibration (70%) and prediction (30%) sets. Model validation employed the coefficient of determination (R^2), root mean square error (RMSE), and ratio of performance to deviation (RPD) as metrics (Equations (4)–(6)).

$$R^2 = 1 - \frac{\sum_{i=1}^N (p_i - d_i)^2}{\sum_{i=1}^N (\bar{p} - d_i)^2} \quad (4)$$

$$RMSE = \sqrt{\frac{\sum_{i=1}^N (d_i - p_i)^2}{N}} \quad (5)$$

$$RPD = \frac{SD}{RMSE} \quad (6)$$

where d_i and p_i represent the actual and predicted values, respectively, of the i -th component, $\bar{p}$ is the average of the predicted values, N is the number of components, $SD = \sqrt{\frac{1}{1-N} \sum_{i=1}^N (d_i - d_{average})^2}$ is the standard deviation of the measured data, and average is the mean of the reference (measured) data values. The RPD was calculated, and the performance of the regression (estimation) system was classified based on the recommendation value ranges provided [39]. In essence, an RPD value less than 1 indicates a very weak and inaccurate model. If RPD falls between 1 and 1.4, the model is considered weak. A suitable model for evaluation and prediction has an RPD between 1.4 and 1.8. For quantitative accurate predictions, an RPD between 1.8 and 2 is required. A very good model exhibits an RPD between 2 and 2.5, while an RPD greater than 2.5 signifies a great model.

Subsequently, hybrid models combining support vector machines (SVM) with genetic algorithms (GA), particle swarm optimization (PSO), ant colony optimization (ACO), and imperialistic competitive algorithm 1 (ICA) were employed to identify optimal wavelengths [40]. SVM is a robust classification technique that constructs a hyperplane to segregate data points into distinct classes. This hyperplane is positioned to maximize the margin between the closest data points of each class, termed support vectors [41]. SVM is a prominent machine learning (ML) algorithm renowned for its efficacy in discerning intricate patterns within complex datasets, surpassing other ML methods [42]. Applications of SVM encompass handwriting recognition, counterfeit credit card detection, speaker identification, and facial recognition [43].

Genetic algorithms (GAs) are heuristic search and optimization techniques inspired by the process of natural evolution. They have been successfully applied to a wide range of complex real-world problems. Originally conceived based on Darwin's principle of evolution through natural selection, GAs employ a highly abstracted version of these processes to evolve solutions to given problems [44].

Swarm-based algorithms have emerged as a potent family of optimization techniques, drawing inspiration from the collective behaviors observed in social animals. Particle swarm optimization (PSO) is a prominent example, wherein a set of potential solutions, termed particles, navigate the parameter space. Their trajectories are influenced by both their individual performance and that of their neighbors. This swarm concept, rooted in the collaborative actions of animals like birds, fish, ants, bees, and termites, underpins the study of multi-agent distributed intelligence systems. Swarms comprise homogeneous, simple agents executing relatively basic tasks and interacting locally with peers and their environment. Consequently, swarm-based algorithms have gained prominence as a class of nature-inspired, population-based optimization methods [45].

Ant colonies exemplify distributed systems that, despite comprising relatively simple individuals, exhibit remarkably complex social structures. This organizational framework empowers the colony to undertake intricate tasks far surpassing the capabilities of any single ant. The study of these self-organizing ant colonies has captivated computer scientists, as their behavior offers valuable models for addressing optimization and distributed control challenges within complex systems [46].

Similarly to other evolutionary algorithms, the Imperialist Competitive Algorithm (ICA) begins with an initial population. Individuals within this population, termed 'countries', are categorized as either 'colonies' or 'imperialists', collectively forming 'empires'. The core of the ICA is the competitive dynamic between these empires. Through this competition, weaker empires dissolve, while stronger ones acquire their colonies. The ultimate goal of the ICA is to converge on a single, dominant empire where all colonies occupy similar positions and share an identical imperial cost. Applications of the ICA to standard benchmark functions have demonstrated its efficacy in addressing diverse optimization challenges [47].

2.4.3. Modeling Based on Effective Wavelengths

Partial least squares regression (PLSR), multiple linear regression (MLR), and artificial neural network (ANN) models were employed to determine the optimal model for predicting bell pepper quality parameters based on effective wavelengths. As previously discussed, the coefficient of determination (R^2), root mean square error (RMSE), and ratio of performance to deviation (RPD) (Equations (4)–(6)) were utilized to evaluate model performance. Artificial neural networks (ANNs) are computational models inspired by the human brain's information processing capabilities. ANNs learn from data rather than explicit programming, identifying patterns and relationships within the data. A network comprises numerous interconnected processing elements (PEs) or artificial neurons, organized in layers and associated with weights. The network's strength lies in its interconnected structure. Each PE receives weighted inputs, processes them through a transfer function, and generates an output. The network's behavior is defined by the transfer functions of

its neurons, learning rules, and architecture. Weights are adjustable parameters, making ANNs parametric systems. The weighted sum of inputs constitutes the neuron's activation, which is transformed into an output by the transfer function. This function introduces nonlinearity to the network. During training, connections between units are optimized to minimize prediction errors and achieve desired accuracy. Once trained and validated, the network can predict outputs based on new input data.

A multilayer perceptron (MLP) artificial neural network, based on the backpropagation algorithm, was employed for this study. The network architecture comprised an input layer with a number of neurons equal to the effective wavelengths, a single-neuron output layer representing the qualitative property, and one or two hidden layers consisting of 10 neurons each. Data were partitioned into training, validation, and testing sets using a 70%–15%–15% split. As a supervised machine learning algorithm, the MLP was implemented using MATLAB's *nnstart* toolbox. The Levenberg–Marquardt algorithm was selected to optimize network weights due to its efficiency in minimizing error [48]. Data analysis was conducted using The Unscrambler X 10.4 and MATLAB 2022a.

3. Results and Discussion

3.1. Quality Parameters

Table 1 presents the measured quality parameters of three bell pepper varieties: firmness, pH, soluble solids content (SSC), titratable acidity (TA), ascorbic acid, anthocyanin, and total phenol (TP). The table provides mean values, minimums, maximums, and standard deviations for each parameter. The yellow variety demonstrated the highest firmness, pH, and TP levels. Conversely, the orange variety exhibited the maximum values for SSC, ascorbic acid, and anthocyanin. Several studies reported that amounts of quality parameters in peppers fruit are influenced by growth conditions and variety-dependent physiological characteristics [49–52].

Table 1. Quality parameters measured in three bell pepper varieties using standard methods.

	Variety	Firmness (N)	pH	SSC (Brix)	TA (%)	Ascorbic Acid (mg in 100 g)	TP (mg/g)	Anthocyanin (mg/g)
Mean	Red	14.051	4.5263	7.963	7.627	200.49	202.27	1.6294
	Yellow	12.947	4.5437	9.060	8.459	208.36	200.15	1.7149
	Orange	12.229	4.41	10.542	10.811	244.98	262.03	1.165
Minimum	Red	9.213	4.33	6.2	6.4	169.08	165	0.8013
	Yellow	8.212	4.39	7	6.72	151.65	128.64	0.8013
	Orange	6.9	4.3	8.9	6.57	190.48	146.82	0.481
Maximum	Red	19.250	4.77	9.1	9.6	275.88	301.36	3.0451
	Yellow	19.363	4.78	10.40	11.52	299.08	415	2.8849
	Orange	18.625	4.52	12.30	13.44	305.94	333.18	4.007
StDev	Red	2.249	0.0961	0.759	0.733	21.89	31.27	0.4612
	Yellow	2.666	0.0845	0.828	1.062	35.02	52.44	0.5360
	Orange	2.929	0.0534	0.898	3.145	30.42	40.84	0.650

3.2. Vis-NIR Spectra

Vis/NIR absorption spectra for all three bell pepper cultivars are presented in Figure 1A–C. To mitigate noise present at the spectral data's beginning and end, each variety was examined within a distinct spectral range. The cultivars exhibit varying qualitative properties and absorption levels within their respective noise-free spectral regions. In all three varieties, absorption increased or decreased in all samples with a similar trend, which may be affected by the color of the samples [53]. According to Figure 1, there is a clear peak for all spectra around the wavelengths of 920 to 940 nm, which may be caused by the protons absorbed by OH or NH [54].

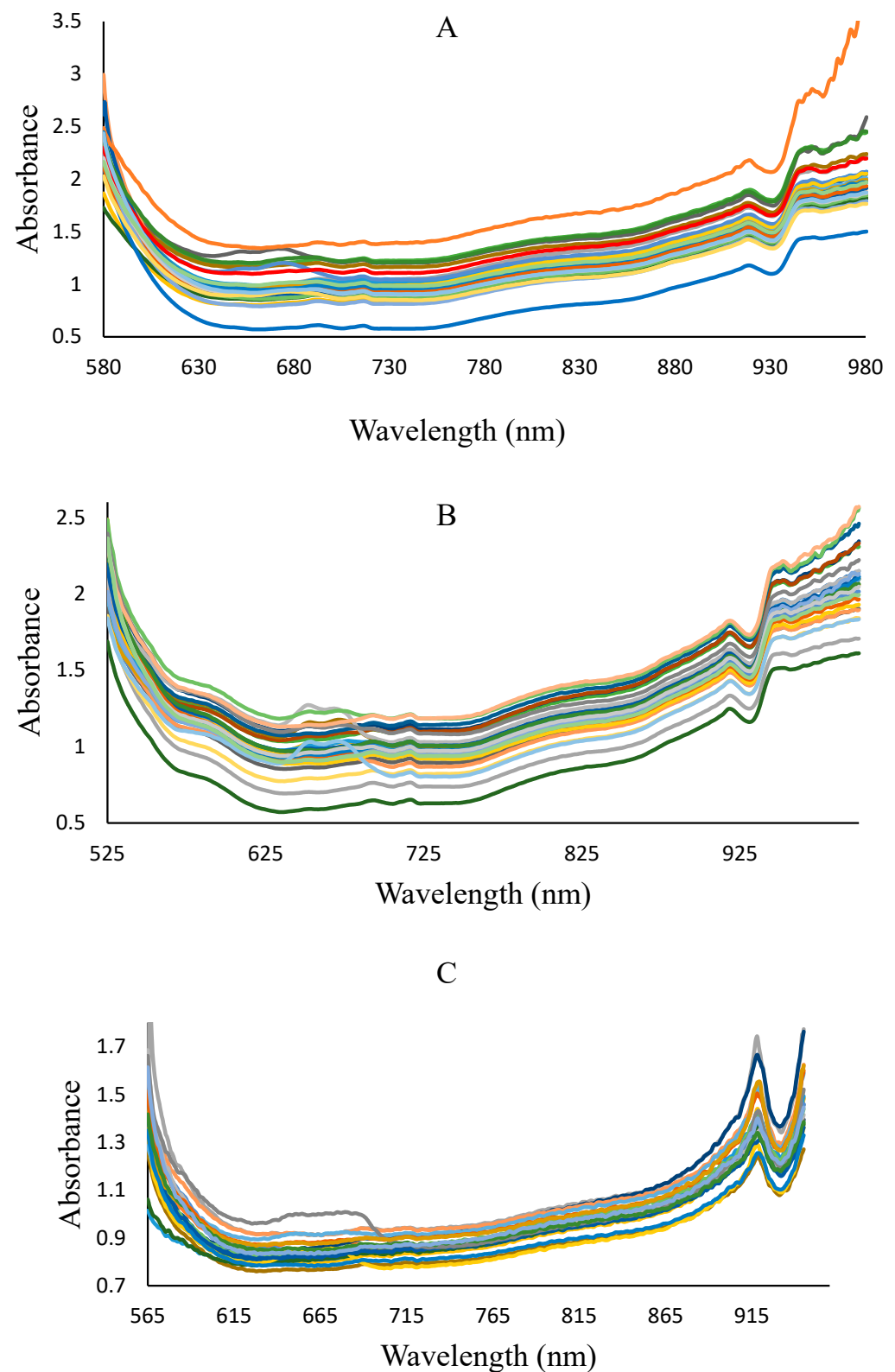


Figure 1. Absorption spectrum of red (A), yellow (B) and orange (C) bell pepper varieties.

3.3. Principal Component Analysis and Outlier Detection

Principal component analysis (PCA) was conducted on the red, yellow, and orange bell pepper samples. As depicted in Figure 2A–C, the first two principal components collectively accounted for 94% and 3%, 94% and 4%, and 74% and 18% of the total variance in the red, yellow, and orange varieties, respectively. Consequently, the first two components

explained 94%, 94%, and 74% of the data variability for the corresponding pepper types. Given the potential influence of technical issues, data collection errors, or inappropriate sampling on the dataset [55,56], outlier detection was performed using Hotelling's T^2 distribution and residual F. The residual F quantifies the distance between a sample and the model, while Hotelling's T^2 indicates how well the model describes the sample [56]. Unscrambler X software facilitated the visualization of outliers as ellipses in the score plot [57]. Outliers can significantly impact analysis results [58]. As shown in Figure 2D,E, one red and two orange bell pepper samples were identified as outliers and subsequently excluded from further analyses. Principal component analysis (PCA) was used to categorize the antioxidant activity of red pepper powder based on near-infrared spectral data [30]. To validate their findings, the researchers opted for full cross-validation, a method known to enhance correlation and statistical power. The results demonstrated the efficacy of this approach in classifying the antioxidant activity of red pepper powder. Variance exceeding 70% for PC1 and PC2 indicates a robust two-dimensional visualization on the score plot [30].

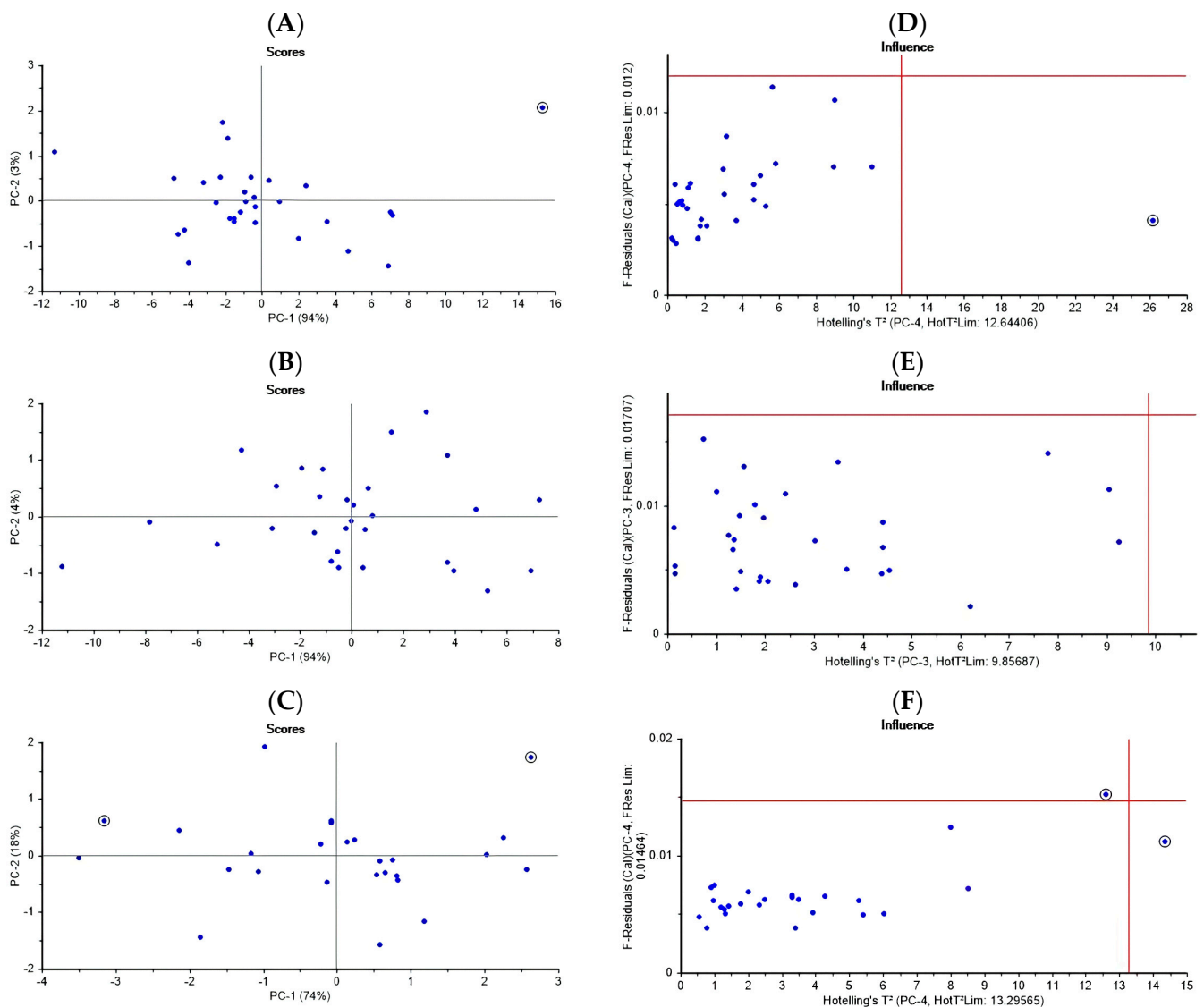


Figure 2. Results of the principal component analysis (PCA) (A–C) and Hotelling's T^2 test (D–F) for red, yellow, and orange varieties, respectively.

3.4. Partial Least Squares (PLS) Regression

Table S1 presents the R^2 , RMSE, and RPD values for calibration and validation sets of the PLS regression model applied to the full dataset. This model effectively predicted the quality properties of red, yellow, and orange varieties, achieving R^2 values exceeding 0.83, 0.58, and 0.73, respectively. These results demonstrate the robust predictive capability of the PLS regression model for all quality parameters across the three varieties. Previous studies have successfully employed NIR spectroscopy for non-destructive assessment of an apple's internal quality. Partial least squares regression (PLSR) models have been developed and validated to predict internal quality attributes, such as total soluble solids (TSSs) and titratable acidity (TA), using external test samples under various conditions [59,60].

Near-infrared spectroscopy (NIRS), combined with partial least squares (PLS) analysis, was used to non-destructively assess antioxidant activity and water content in red pepper powder [27]. The PLS model was developed using Unscrambler X version 11.0 software. Results indicate that the PLS method is precise and holds promise for quantifying antioxidant activity and water content in red pepper powder samples [27].

3.5. Effective Wavelengths

Support vector machine (SVM) models combined with genetic algorithm (GA), particle swarm optimization (PSO), ant colony optimization (ACO), and Imperialist Competitive Algorithm (ICA) were employed to determine effective wavelengths for different bell pepper varieties. Based on average correlation, mean squared error (MSE), and relative percent difference (RPD), an average of 15 effective wavelengths were identified per variety. The following parameter settings were used for wavelength selection: GA (population size: 120, generations: 10, crossover rate: 30%, mutation rate: 30%), PSO (particle count: 40, iterations: 10, personal best count: 8), ACO (ant count: 40, iterations: 10, evaporation rate: 4), and ICA (country count: 40, imperialism count: 11). Algorithm performance was evaluated using average convergence of mean RMSE, average correlation, and RPD across all samples. Convergence indicates improved results with increased iterations or computational time. Figures 3–9 and Table S2 present Feature Select outputs for quality parameters of the three studied varieties based on these criteria. PSO and ACO demonstrated decreasing average RMSE and satisfactory average correlation convergence. Considering computational efficiency, with ACO requiring more time, PSO emerges as the preferred method among the four algorithms. These findings align with previous research on effective wavelength determination for polyphenol oxidase and peroxidase enzyme activity detection in bell peppers [61]. In another study [62], visible/near-infrared (Vis/NIR) spectroscopy to assess the viability of two peanut seed types was used. To optimize wavelength selection for this assessment, they applied a variety of meta-heuristic algorithms, including World Competitive Competition (WCC), League Championship Algorithm (LCA), Genetics (GA), particle swarm optimization (PSO), ant colony optimization (ACO), Imperial Competitive Algorithm (ICA), Learning Automata (LA), Heat Transfer Optimization (HTS), Forest Optimization (FOA), Discrete Symbiotic Search (DSOS), and Cuckoo Optimization (CUK). These algorithms effectively extracted wavelength-related information from the spectral data. Notably, all algorithms demonstrated high accuracy in predicting the allometric coefficient of the seeds, achieving correlation coefficients exceeding 0.985 and errors below 0.0036. Tables S3–S5 present the effective wavelengths for red, yellow, and orange varieties, ranked by their influence on quality parameters. Wavelengths determined using the SVM-PSO method reveal spectral bands with consistent positions and shapes but notable intensity fluctuations. These bands are likely associated with the overtones and combination tones of hydrogen-containing structural groups, predominantly O–H and C–H. Originating primarily from the C–H and O–H groups within fruit constituents, these absorptions may be attributed to various compounds, including water, sugars, other carbohydrates, organic acids, polyphenols, certain vitamins, and specific amino acids [63].

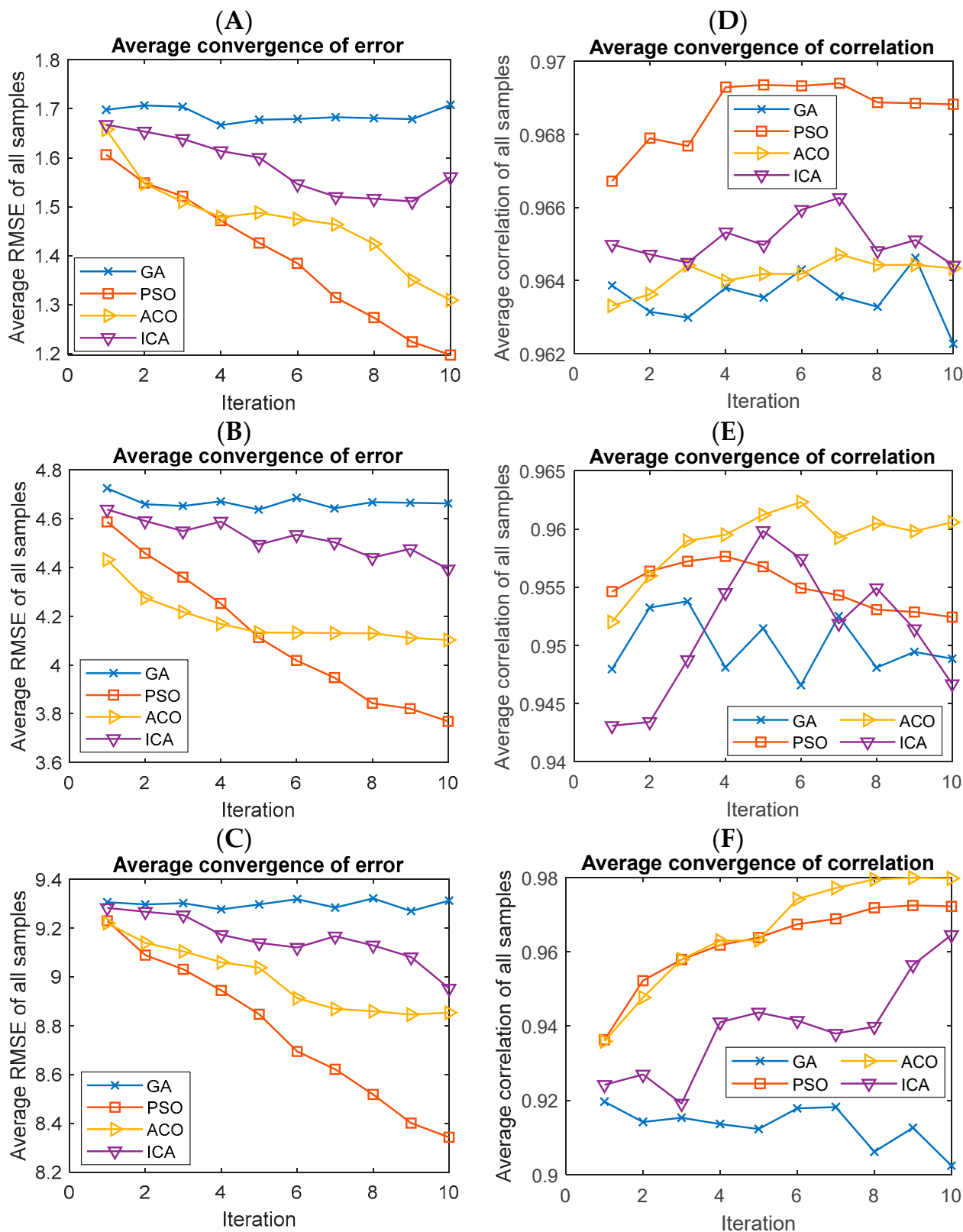


Figure 3. The firmness of the three bell pepper varieties using SVM. These diagrams compare the performance of algorithms in terms of accuracy and error score. RMSE variations (A–C) and average correlation (D–F) for red, yellow, and orange varieties, respectively.

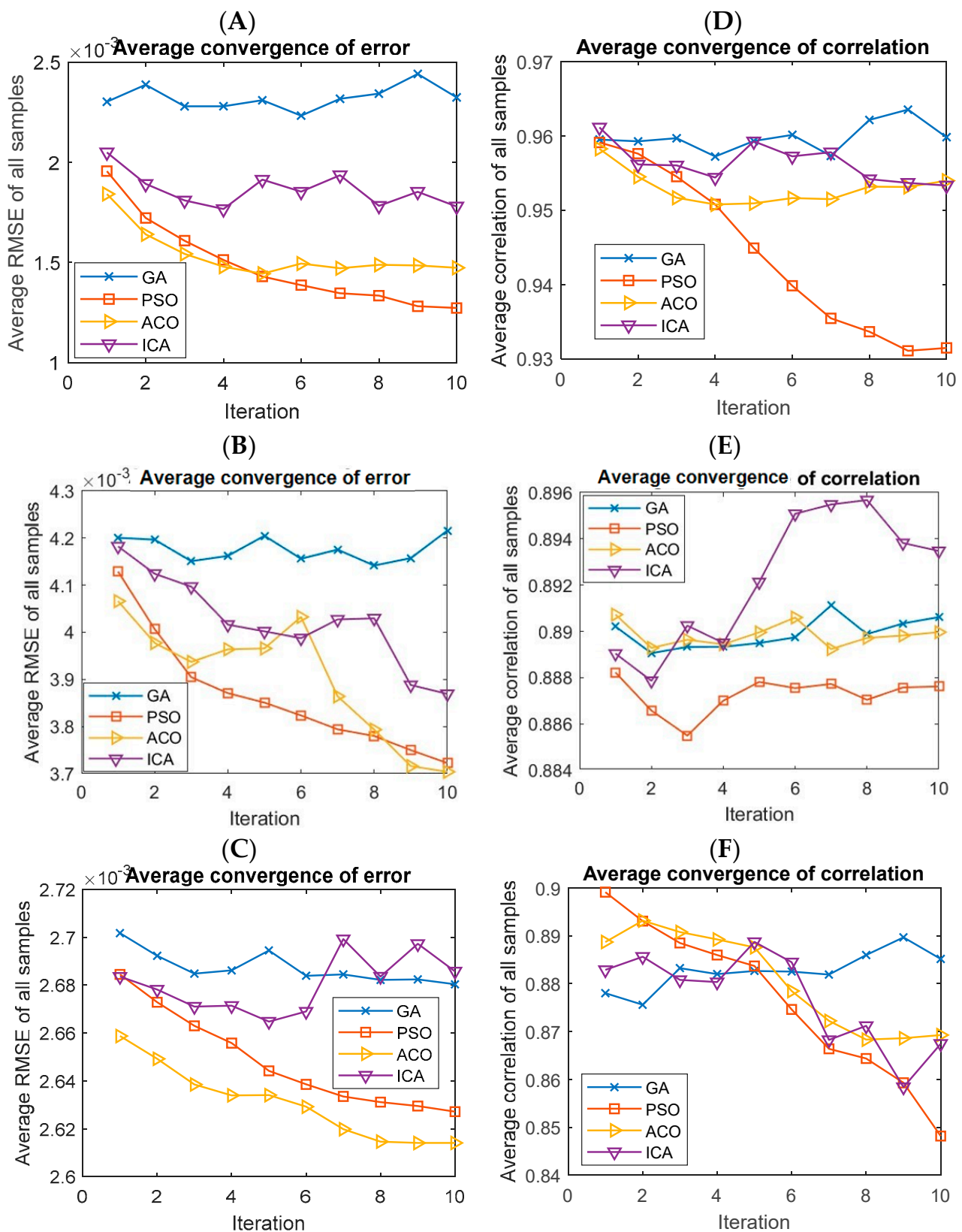


Figure 4. The pH of the three bell pepper varieties using SVM. These diagrams compare the performance of algorithms in terms of accuracy and error score. RMSE variations (A–C) and average correlation (D–F) for red, yellow, and orange varieties, respectively.

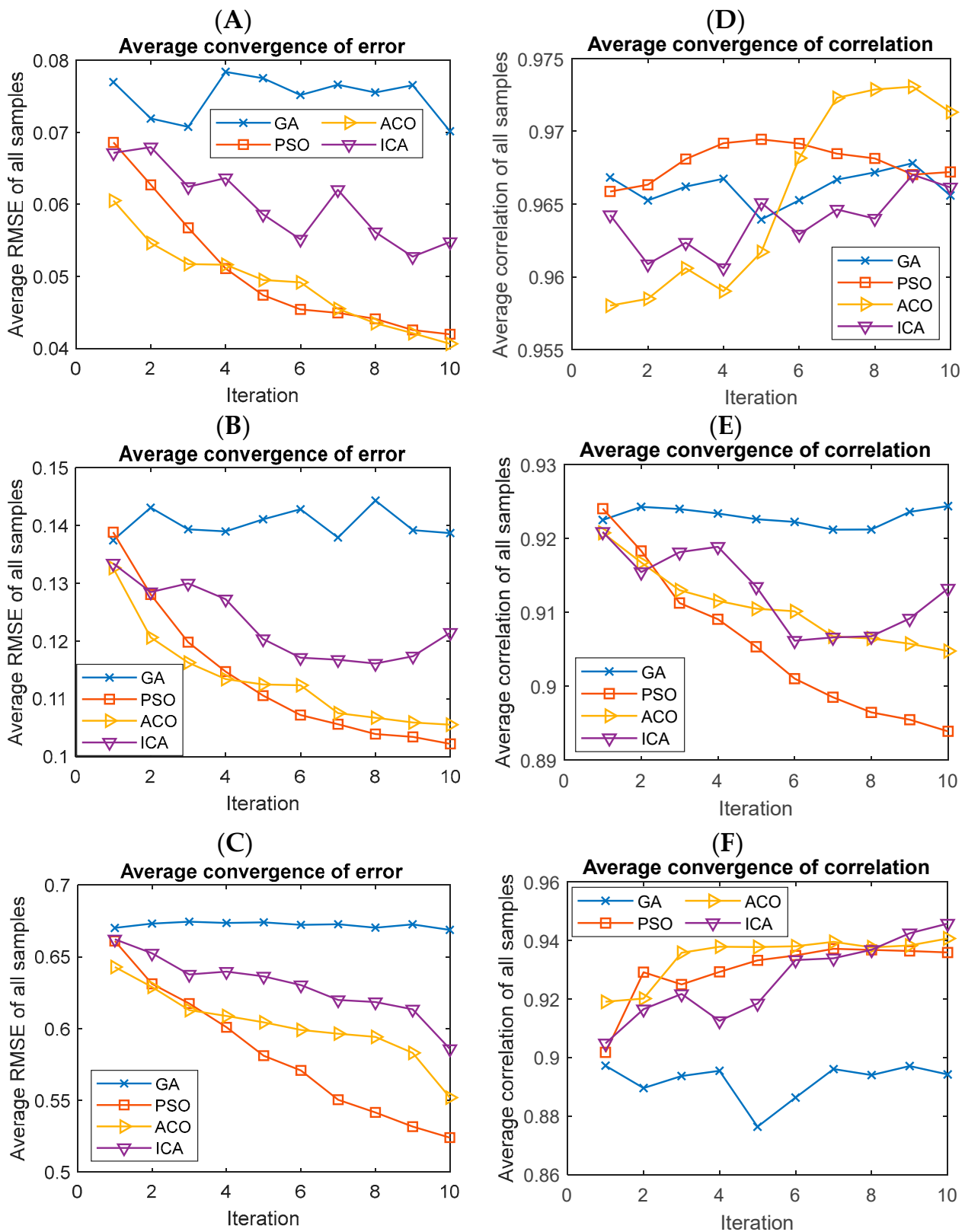


Figure 5. The SSC of the three bell pepper varieties using SVM. These diagrams compare the performance of algorithms in terms of accuracy and error score. RMSE variations (A–C) and average correlation (D–F) for red, yellow, and orange varieties, respectively.

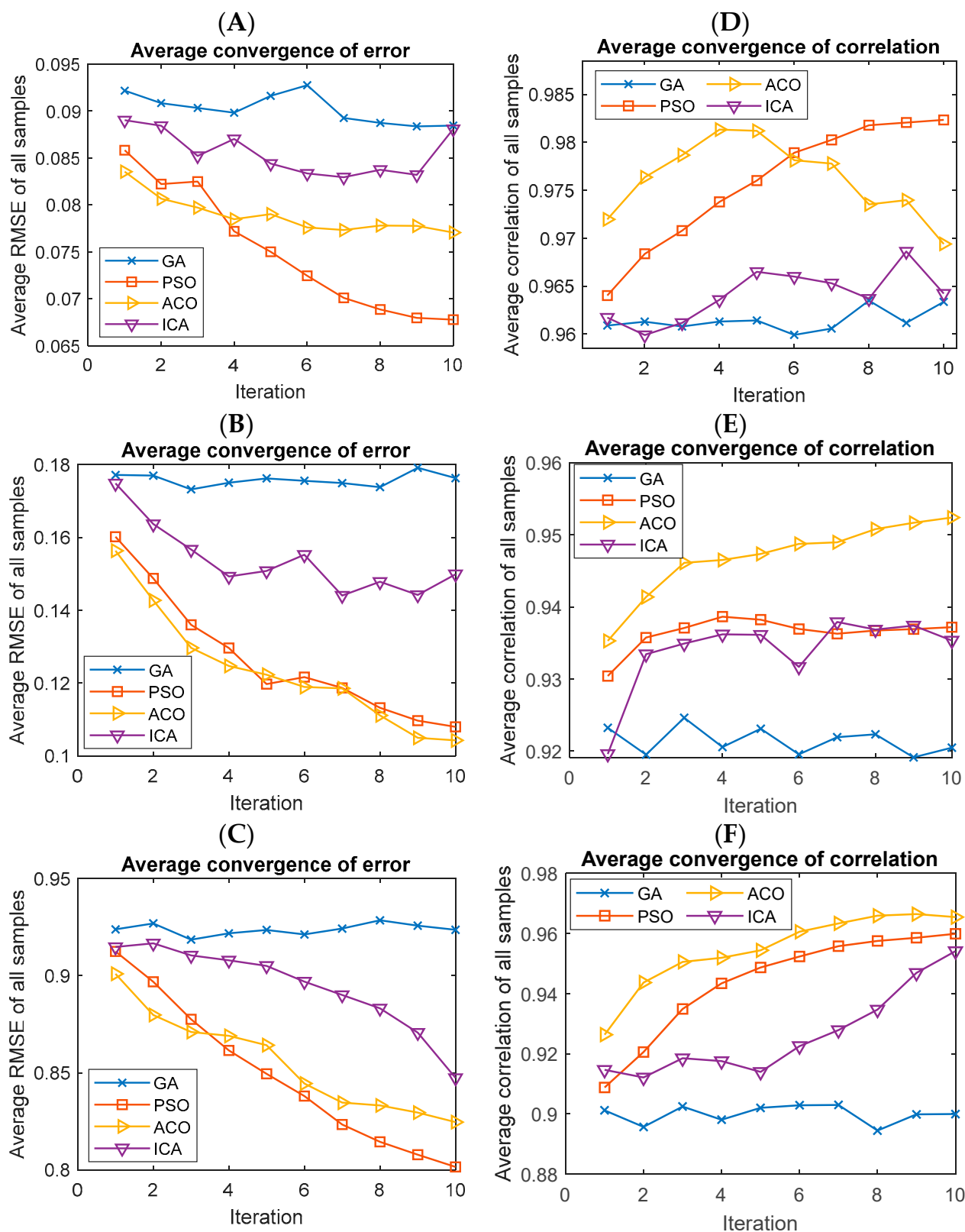


Figure 6. The TA of the three bell pepper varieties using SVM. These diagrams compare the performance of algorithms in terms of accuracy and error score. RMSE variations (A–C) and average correlation (D–F) for red, yellow, and orange varieties, respectively.

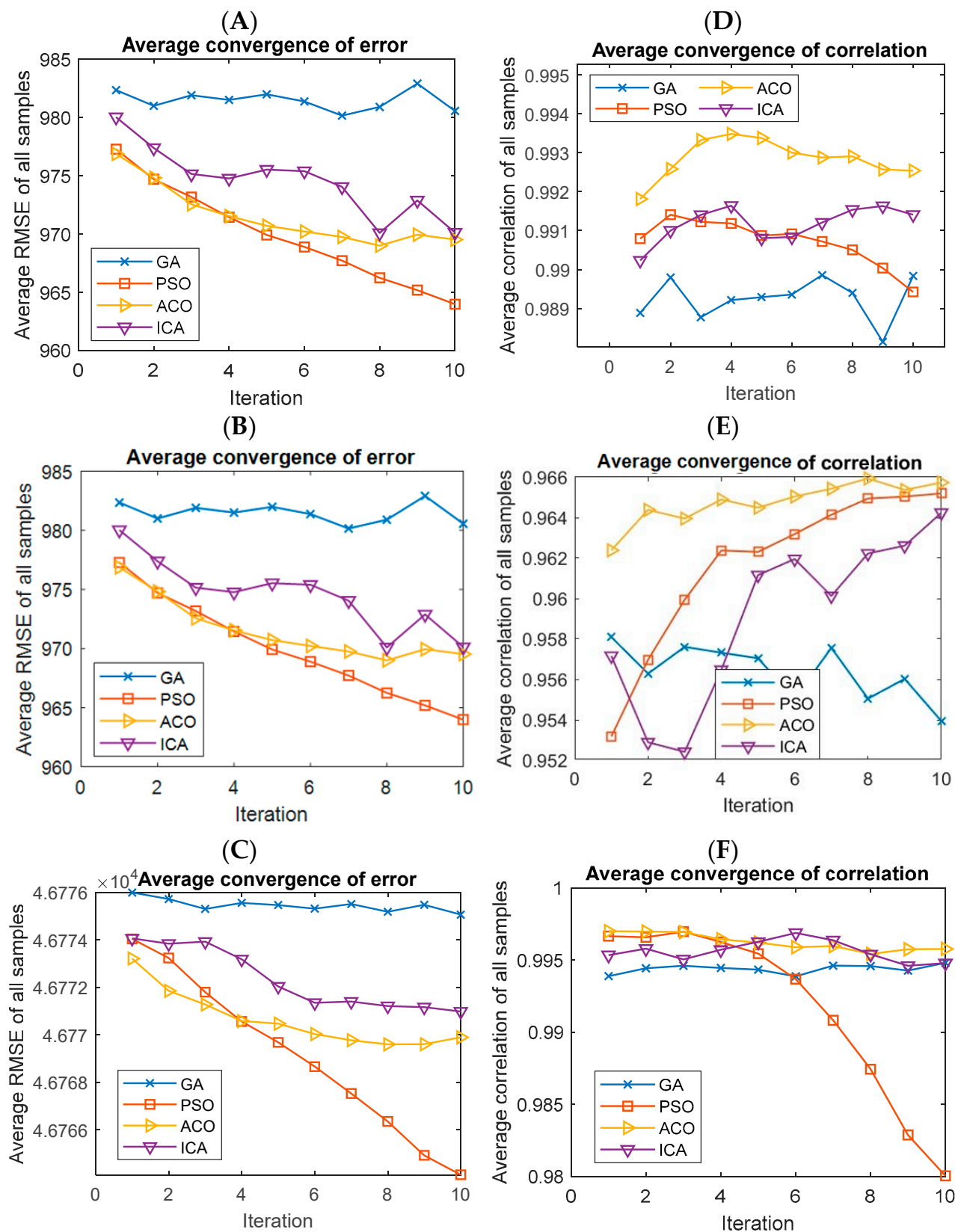


Figure 7. The vitamin C content of the three bell pepper varieties using SVM. These diagrams compare the performance of algorithms in terms of accuracy and error score. RMSE variations (A–C) and average correlation (D–F) for red, yellow, and orange varieties, respectively.

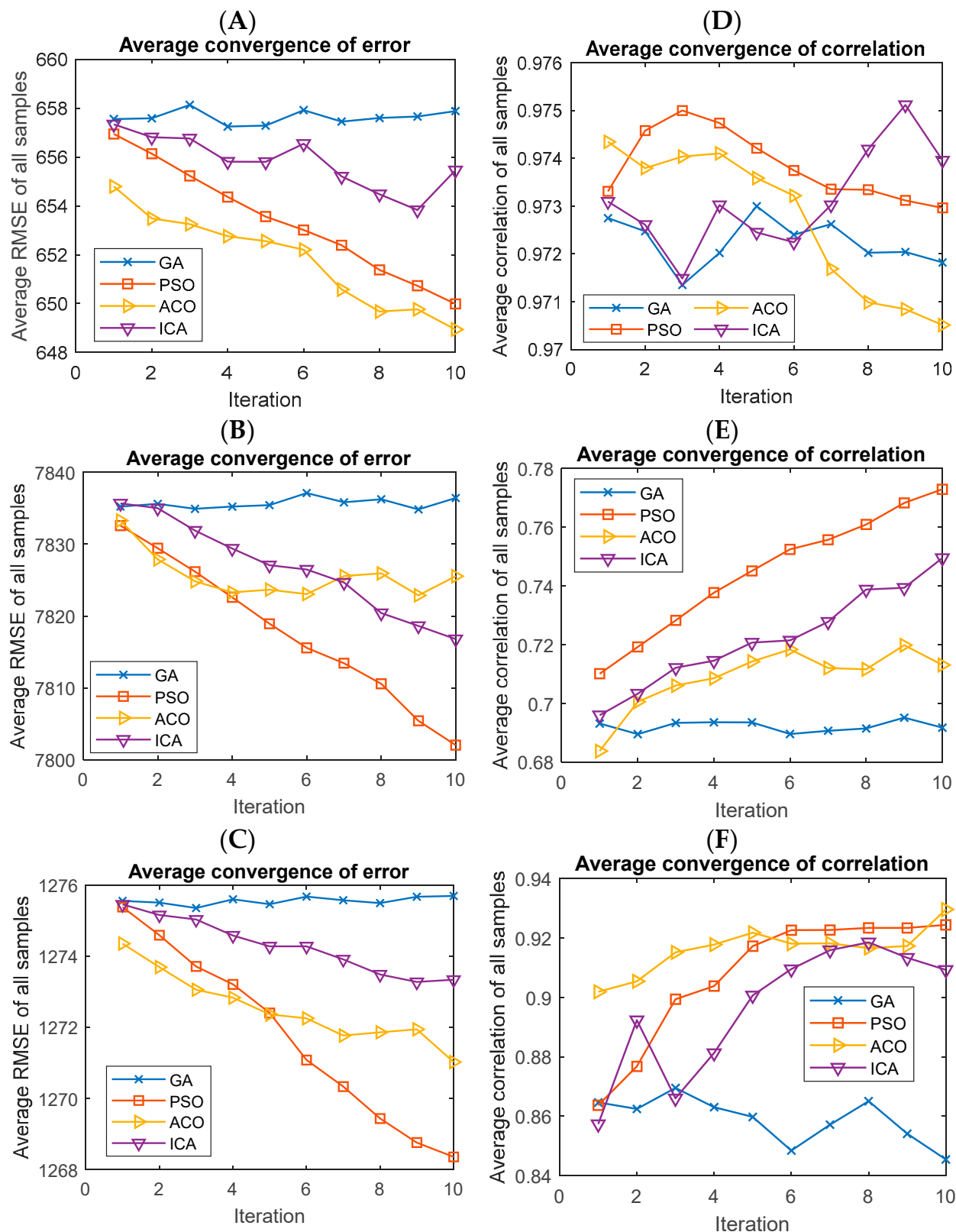


Figure 8. The total phenol content of the three bell pepper varieties using SVM. These diagrams compare the performance of algorithms in terms of accuracy and error score. RMSE variations (A–C) and average correlation (D–F) for red, yellow, and orange varieties, respectively.

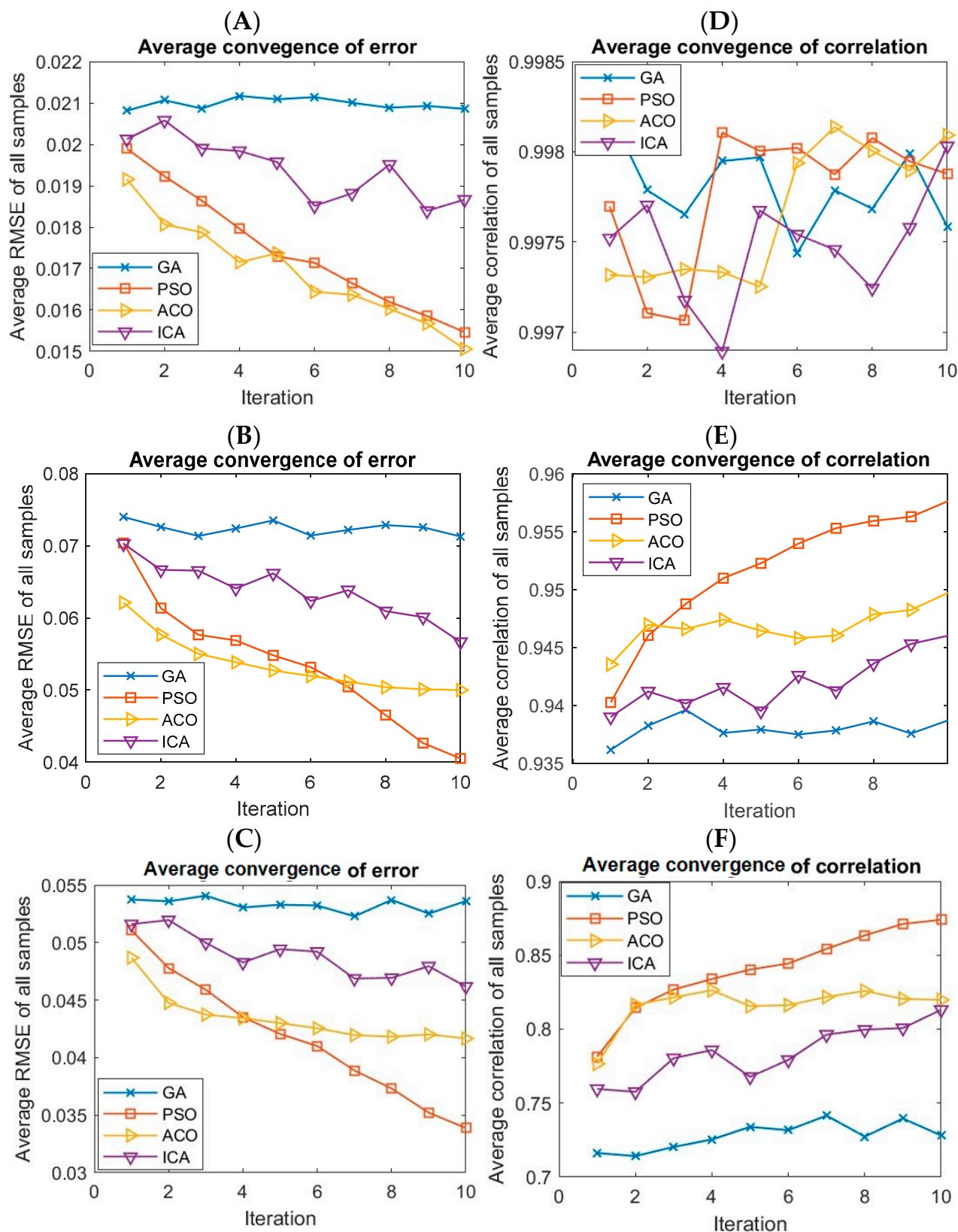


Figure 9. The anthocyanin content of the three bell pepper varieties using SVM. These diagrams compare the performance of algorithms in terms of accuracy and error score. RMSE variations (A–C) and average correlation (D–F) for red, yellow, and orange varieties, respectively.

Based on the literature data, spectral bands within specific ranges are associated with various biochemical components in bell peppers. Bands at 700–800 nm (third overtone of O–H from carboxylic and enediol acids) and 800–900 nm (second overtone O–H from carboxylic and enediol acids) are potentially linked to pH, titratable acidity (e.g., malic acid), and vitamin C content (as an enediol acid). Additionally, the region near 910–930 nm, attributed to C–H stretching from carboxylic acids [59,64], is likely related to these parameters as well. Bands near 768 nm (fourth overtone of C–H) and 986 nm (second overtone of O–H) are associated with sample pH [65]. Given the absence of organic acids in the 600–700 nm range [64], it is probable that spectral features in this region primarily reflect the color of bell peppers. Furthermore, the 921–1039 nm range ($9622\text{--}10,854\text{ cm}^{-1}$), particularly at 938, 938.5, and 998 nm, falls within the third-order overtone band of OH groups associated with cellulose [66] and, consequently, firmness [67]. Notably, specific wavelengths within this range (978.5 and 975 nm, 929 and 999.5 nm, and 930.5 and 924 nm) were identified as crucial for estimating total phenols and anthocyanins in red, yellow, and orange bell peppers, respectively, using SVM-PSO [68,69]. These findings suggest a correlation between this spectral region and the content of phenols and anthocyanins, compounds containing one or more hydroxyl groups (O–H). Finally, wavelengths between 550 and 750 nm are likely influenced by variations in anthocyanin and chlorophyll concentrations [54]. Wavelengths within the 950–1075 nm range (encompassing the second and third overtones of O–H and C–H vibrations) and near 910 nm (third overtone band of O–H), specifically 911, 949, 956.5, 959.5, 975.5, 976, 988, 991.5, 999, and 1000 nm, have been identified as particularly important for detecting the soluble solid content (SSC) of bell peppers using SVM-PSO. These wavelengths may also be crucial for SSC calibration [59,70]. Wavelengths around 700 and 950 nm (specifically 700, 700.5, 701, 949, 949.5, and 951.5 nm in their study) likely correspond to the third overtone stretch of C–H and the second and third overtones of O–H in water [71]. Additionally, a strong absorption peak near 975 nm (attributed to the second overtone of O–H) was associated with water and carbohydrates [72]. As each wavelength carries complex information about various compounds, isolating the composition of a specific substance solely based on these wavelengths proves challenging. Consequently, data analysis becomes indispensable for uncovering the hidden relationship between spectral data and qualitative properties.

3.6. Modeling Based on the Effective Wavelength

PLSR, MLR, and ANN methods were employed to model the SVM-PSO-selected effective wavelengths. Table S6 presents the R^2 (coefficient of determination), RMSE (root mean square error), and RPD (ratio of performance to deviation) values for the calibration and validation of PLSR and MLR models, respectively. Table S7 displays the corresponding values for the training, validation, and testing phases of the ANN model. The ANN model consistently outperformed PLSR and MLR in terms of validation R^2 , RMSE, and RPD for all quality properties across the different bell pepper varieties. Specifically, the ANN model achieved the highest R^2 and RPD values (0.99 and 314.5, respectively) for total acidity (TA) in red and orange varieties, while recording the lowest RMSE (0.010677) for pH in the red variety. These results indicate that while all models developed using effective wavelengths demonstrated acceptable accuracy in predicting bell pepper quality characteristics, the ANN model exhibited superior predictive performance. This superiority can be attributed to the ANN's ability to learn directly from data without requiring the estimation of statistical characteristics, as reported in numerous studies across various fields [13,61,73]. A study utilized PLS and ANN methods for non-destructive, real-time monitoring of apple firmness during ultrasonic contact drying [74]. Employing portable NIR spectroscopy, they evaluated model performance using output cross-validation and an external dataset. To explore the impact of spectral changes on stiffness prediction, several pre-treatments were applied. Through weighted regression coefficients, seven significant wavelengths were identified and used to construct a simple MLR model for enhanced interpretability and noise reduction. Models incorporating PLS, MLR, and ANN with

selected wavelengths predicted apple hardness with R^2 p values of 0.91, 0.91, and 0.95, respectively, and RMSEP values of 14.78 N, 14.85 N, and 12.46 N. These results demonstrate the superior performance of the ANN method compared to PLS and MLR [74]. Authors in another study applied a genetic algorithm neural network (GANN) to near-infrared spectral data for classifying oil palm ripeness [75]. Their findings revealed that the GA effectively reduced learning time and optimized the NN architecture by systematically minimizing identification errors and circumventing the conventional iterative approach. Dimensionality reduction through PCA generated new component variables, accelerating the GANN data analysis process and facilitating the identification of optimal solutions.

4. Conclusions

This study employed Vis-NIR spectroscopy in absorbance mode for the non-destructive evaluation of quality properties in three bell pepper varieties within the spectral range of 350–1150 nm. To enhance data analysis, principal component analysis (PCA) was used for dimensionality reduction, and Hotelling's T^2 test identified outliers. Partial least squares (PLS) regression determined the optimal model for the full dataset. To identify effective wavelengths, the support vector machine (SVM) method was combined with genetic algorithm (GA), particle swarm optimization (PSO), ant colony optimization (ACO), and independent component analysis (ICA) metaheuristic optimization techniques. Subsequently, PLS, multiple linear regression (MLR), and artificial neural networks (ANNs) were employed for modeling using the selected wavelengths. Each algorithm identified an average of 15 wavelengths. SVM-PSO was chosen for non-destructive quality evaluation based on its superior correlation, fewer selected wavelengths, and faster computation time. While ANN exhibited the best performance in terms of validation R^2 , root mean square error (RMSE), and relative prediction deviation (RPD), it was selected as the optimal prediction model. This research demonstrates the practical applicability of combining Vis/NIR spectroscopy with ANN and SVM-PSO variable selection for non-destructive quality evaluation in vegetables. The identified effective wavelengths hold potential for designing or optimizing spectroscopic instruments to predict quality properties in bell peppers.

Supplementary Materials: The following supporting information can be downloaded at: <https://www.mdpi.com/article/10.3390/app142310855/s1>, Table S1: R^2 , RMSE and RPD values for calibration and validation sets of the regression model; Table S2: Average values of correlation, RMSE and RPD of meta-heuristic algorithms; Table S3: Effective wavelengths of the red varieties determined by different algorithms; Table S4: Effective wavelengths of the yellow varieties determined by different algorithms; Table S5: Effective wavelengths of the orange varieties determined by different algorithms; Table S6: R^2 , RMSE and RPD value of the calibration and validation datasets of PLSR and MLR methods created based on the effective wavelengths; Table S7: R^2 , RMSE and RPD value of the training and validation datasets of ANN method created based on the effective wavelengths.

Author Contributions: M.L.A.: Conceptualization, data curation, data analysis and writing—original draft preparation; Y.A.-G.: Investigation, supervision, conceptualization, data curation, data analysis and writing—original draft preparation; M.T. and M.K.: Methodology, validation, writing—review and editing, and investigation; H.S.E.-M.: Methodology, validation, writing—review and editing, and investigation; M.S. (Maciej Sprawka): Investigation, resources, funding acquisition, writing—review and editing; M.S. (Mariusz Szymanek): Formal analysis, resources, funding acquisition, project administration and writing—review and editing. All authors have read and agreed to the published version of the manuscript.

Funding: This research received no specific grant from any funding agency in the public, commercial, or not-for-profit sectors.

Institutional Review Board Statement: Not applicable.

Informed Consent Statement: Not applicable.

Data Availability Statement: All data and materials are available upon reasonable request from the corresponding author.

Conflicts of Interest: The authors declare no conflicts of interest.

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